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|----------|---|
|          | WEDNESDAY   |
|          | OMICS: QUANTITATION TECHNIQUES, 001 - 034   |
| WP 001   | Use of iTRAQ and MudPIT to Quantify Synaptic  |
|          | Protein Expression Changes in Post-Synaptic Density Isolated from Individual Mouse Brains; Zhongping Liao; Yunhu Wan; Sarah Rynarzewski; Stefani Thomas; Austin J. Yang; Univ of Maryland Baltimore, Baltimore, MD  |
| WP 002   | Identification of Potential Kidney Stem Cell Markers  |
|          | using Quantitative Proteomics; Lorraine Anderson <sup>1</sup> ; Md Abedin <sup>1</sup> ; Pratik Jagtap <sup>2</sup> ; Sunayan Bandyopadhyay <sup>1</sup> ; Chad Myers <sup>1</sup> ; Raj Kasthuri <sup>3</sup> ; Sandeep Gupta <sup>1</sup> ; <sup>1</sup> University of Minnesota, Minneapolis, MN; <sup>2</sup> Minnesota Supercomp. Inst., Minneapolis, MN; <sup>3</sup> University of   |
|          | North Carolina at Chapel Hill, Chapel Hill, NC  |
| WP 003   | Discovery of New Lysosomal Protein Candidates by iTRAQ 8-Plex Analysis of Rat Liver Gradient Fractions; Maria Cecilia Della Valle <sup>1</sup> ; Michel Jadot <sup>2</sup> ; Haiyan Zheng <sup>1</sup> ; David E. Sleat <sup>1</sup> ; Peter Lobel <sup>1</sup> ; <sup>1</sup> CABM/UMDNJ, Piscataway, NJ; <sup>2</sup> Facultes  |
| ****     | Universitaires Notre-Dame de la Paix, Namur, Belgium  |
| WP 004   | Quantitative Proteomic Analysis Of Mycobacterium<br>Semegmatis by iTRAQ labeling and LC/MALDI-<br>TOF-TOF; Fa-yun Che; Eleanor Russell Goldman;<br>Edward Nieves; John Chan; Ruth Hogue Angeletti;<br>Albert Einstein College of Medicine, Bronx, NY  |
| WP 005   | Identification of New Markers of Mesenchymal Stem   |
| WP 006   | Cell Differentiation with iTRAQ® Technology; Leeann Higgins; Troy C. Lund; Lorraine Anderson; Amanda J. Kobs; Paul J. Orchard; Jakub Tolar; University of Minnesota, Minneapolis, MN  Is Diversity Library Dynamic Range Leveling a Valid   |
| W P 000  | Approach for Quantitative Proteomics? <u>Lashanda N.</u> <u>Waller;</u> Susana Comte-Walters; Daniel R. Knapp; <i>Medical University of SC, Charleston, SC</i>  |
| WP 007   | Validation of Protein Quantification Strategies for   |
| NID 222  | Complex Samples: Comparison of iTRAQ and Multiple Reaction Monitoring (MRM) Quantitation Schemes; Gregg A. Czerwieniec; Jason M. Held; Sung W. Choi; Birgit Schilling; Simon Melov; Bradford W. Gibson; Buck Institute for Age Research, Novato, CA   |
| WP 008   | Tandem Mass Tags for Selection and Absolute   |
|          | Quantification of Brain Damage Markers in CSF;<br><u>Loïc Dayon</u> <sup>1</sup> ; Natacha Turck <sup>1</sup> ; Alexander Scherl <sup>1</sup> ; Stefan<br>Kienle <sup>2</sup> ; Jean-Charles Sanchez <sup>1</sup> ; <sup>1</sup> Geneva University,<br>Geneva, Switzerland; <sup>2</sup> Proteome Sciences R&D GmbH<br>& Co. KG, Frankfurt am Main, Germany   |
| WP 009   | Candidate Verification of Iron-Sensitive  |
|          | Meningococcal Proteins Using TMT SRM; Helen<br>Byers <sup>1</sup> ; James Campbell <sup>1</sup> ; Karsten Kuhn <sup>2</sup> ; Malcolm<br>Ward <sup>1</sup> ; Peter Schulz-knappe <sup>2</sup> ; Peter van Ulsen <sup>3</sup> ; Jan<br>Tommassen <sup>3</sup> ; Thorsten Prinz <sup>2</sup> ; <sup>1</sup> Proteome sciences plc,<br>London, UK; <sup>2</sup> Proteome Sciences R&D, Frankfurt/<br>Main, Germany; <sup>3</sup> University of Utrecht, Utrecht, |
| WD 010   | Holland   |
| WP 010   | Age Dependent Changes in the Mitochondrial  |

Proteome of APP/PS1 Transgenic Mice; You-Jun Fu;

Shuling Xiong; Mark A Lovell; Bert C Lynn; University

Networks in Mouse Heart; Cexiong Fu; Changgong

**Maturation of Toxins in the Venom Duct of Conus** 

Gilles<sup>2</sup>; Stéphanie Kirsch<sup>1</sup>; Edwin De Pauw<sup>1</sup>; Loic

Textile; Rowan L. Dobson<sup>1</sup>; Mike Collodoro<sup>1</sup>; Nicolas

Wu; Tong Liu; Tetsuro Ago; Peiyong Zhai; Junichi

**Elucidation of Thioredoxin Targeted Protein** 

Sadoshima; Hong Li; UMDNJ, Newark, NJ

of Kentucky, Lexington, KY

WP 011

WP 012

- Y POSTERS Ouinton<sup>1</sup>; <sup>1</sup>Liege University, Liege, Belgium; <sup>2</sup>CEA Saclay, Gif sur Yvette, France WP 013 **Quantitative Proteomic Analysis in Transformed Astrocytes Using Spectral Counting and SILAC** Methods; Kiyonaga Fujii<sup>1</sup>; Ken Sasai<sup>2</sup>; Taichi Kimura<sup>2</sup>; Shinya Tanaka<sup>2</sup>; Fuyuhiko Inagaki<sup>1</sup>; <sup>1</sup>Hokkaido University, Sapporo, Japan; <sup>2</sup>Hokkaido University Graduate School of Medicine, Sapporo, Japan WP 014 **Comparative Analyses of Proteins from Two Distinct Bacterial Populations Using SILAC**; <u>Deborah Post</u><sup>1</sup>; Margaret Ketterer<sup>2</sup>; Jason Johnston<sup>2</sup>; Michael Apicella<sup>2</sup>; Bradford W. Gibson<sup>1</sup>; <sup>1</sup>Buck Institute, Novato, CA; <sup>2</sup>The University of Iowa, Iowa City, IA WP 015 **Evaluating the Protein Stoichiometry within Protein-**RNA Complexes by Multiple Reaction Monitoring in Comparison to MS Standard Methods; Carla Schmidt<sup>1</sup>; Michael Grote<sup>3</sup>; Christof Lenz<sup>2</sup>; Reinhard Lührmann<sup>3</sup>; Henning Urlaub<sup>1</sup>; <sup>1</sup>MPI for Biophysical Chemistry, Bioanalytical MS, Göttingen, Germany; <sup>2</sup>PSM Support, Applied Biosystems, Darmstadt, Germany; <sup>3</sup>MPI for Biophysical Chemistry, Cell. Biochemistry, Göttingen, Germany WP 016 A Comparison of Analytical Approaches to the **Detection and Quantitation of Proteins in Complex** Biological Matrices; Anita Izrael-Tomasevic; Lilian Phu; Qui Phung; Jennie Lill; David Arnott; Genentech, Inc., South San Francisco, CA WP 017 **Quantitative Mitochondrial Proteome of Pancreatic** INS-1ß Cells Stimulated with Prolonged High Glucose Using SILAC; Xiulan Chen; Ziyou Cui; Junjie Hou; Zhensheng Xie; Peng Xue; Jing Li; Peng Wu; Linan Shi; Tanxi Cai; Fuquan Yang; Institute of Biophysics, CAS, Beijing, China WP 018 **Protein Profiles of Cisplatin Treated CEM Cells - An Interesting Insight from Three Different Techniques**; Petr Novak<sup>1,5</sup>; Petr Pompach<sup>1,5</sup>; Petr Man<sup>1</sup>; Martin Strohalm<sup>1,2</sup>; Vladimir Havlicek<sup>1,4</sup>; Jirina Martinkova<sup>3</sup>; Hana Kovarova<sup>3</sup>; Petr Dzubak<sup>4</sup>; Marian Hajduch<sup>4</sup>; <sup>1</sup>Institute of Microbiology, Prague 4, Czech Republic; <sup>2</sup>Institute of Chemical Technology, Prague, Czech Republic; <sup>3</sup>Intitute of Animal Physiology and Genetics,, Libechov, Czech Republic; <sup>4</sup>Palacky University, Olomouc, Czech Republic; 5Charles University, Prague, Czech Republic WP 019 Proteome-Wide Quantitative Mass Spectrometry of Astrocyte Protein Secretion; Todd M. Greco; Lynn A. Spruce; Adrian Mak; Steven H. Seeholzer; Harry Ischiropoulos; Children's Hospital of Philadelphia, Philadelphia, PA WP 020 Can Quantitative Proteomics Predict the Effects of **Autophagy Inhibition on Mitochondrial Function?** Rongxiao Sa; Marian Navratil; Xin Xu; Edgar A. Arriaga; University of Minnesota, Minnespolis, MN WP 021 Stoichiometry and Absolute Quantification of Ribosomal Proteins by Mass Spectrometry using
  - QconCAT Technology; Zubida Al-Majdoub; Simon J. Gaskell; Jill Barber; University of Manchester, Manchester, UK
  - WP 022 **Determination of Clp Protease Complex Composition** in Arabidopsis Thaliana Chloroplasts by Quantitative Mass Spectrometry; Paul Dominic B. Olinares<sup>1</sup>; Boris Zybailov<sup>1</sup>; Qi Sun<sup>2</sup>; Klaas J. Van Wijk<sup>1</sup>; <sup>1</sup>Plant Biology, Cornell University, Ithaca, NY; <sup>2</sup>Computational Biology Unit, Cornell University, Ithaca, NY

- WP 023 Circadian Differences of Photoreceptor Outer
  Segment Proteome Observed by Proteolytic <sup>18</sup>O
  Labeling; Dagmar Hajkova<sup>1</sup>; Chao Yuan<sup>2</sup>; Masaru
  Miyagi<sup>3</sup>; <sup>1</sup>Case Western Reserve Univ, Cleveland, OH;
  <sup>2</sup>Case Western Reserve Univ., Cleveland, OH; <sup>3</sup>Case
  Western Reserve Univers, Cleveland, OH
- WP 024 18O Labeling and Mass Spectrometry as a Simple Tool for High Confidence Protein-Protein Interaction Analysis; Karel Bezstarosti; Alireza Ghamari; Frank Grosveld; Jeroen Demmers; Erasmus Medical Center, Rotterdam, Netherlands
- WP 025 Quantitative Proteomic Elucidation of the Core
  AAA+ Vacuolar Protein Sorting 4B ATPase Protein
  Interaction Complex; Stefani N. Thomas<sup>1</sup>; Yunhu
  Wan<sup>1</sup>; Zhongping Liao<sup>1</sup>; David K. Ann<sup>2</sup>; Phyllis I.
  Hanson<sup>3</sup>; Austin J. Yang<sup>1</sup>; <sup>1</sup>Univ of Maryland Baltimore,
  Baltimore, MD; <sup>2</sup>City of Hope, Duarte, CA; <sup>3</sup>Washington
  University, St. Louis, MO
- WP 026 Discovery of Disease-Related Proteins in the Min Mouse Model for Colorectal Cancer via <sup>15</sup>N Metabolic Labeling and Microarray Analysis; Edward L. Huttlin<sup>1,2</sup>; Xiaodi Chen<sup>1</sup>; Gregory Barrett-Wilt<sup>1</sup>; Richard Halberg<sup>1</sup>; Adrian D. Hegeman<sup>3</sup>; Melanie M. Ivancic<sup>1</sup>; Michael A. Newton<sup>1</sup>; Amy C. Harms<sup>1</sup>; William F. Dove<sup>1</sup>; Michael R. Sussman<sup>1</sup>; <sup>1</sup>University of Wisconsin, Madison, WI; <sup>2</sup>Harvard Medical School, Boston, MA; <sup>3</sup>University of Minnesota, Saint Paul, MN
- WP 027 The Role of Nascent Peptide-Ribosome Interactions in Gene Regulation Using Quantitative Mass Spectrometry with 15N-Stable Isotope Labeling;

  Blanca Martínez-Garriga; Hua Xu; Krishna Kannan;
  Alexander Mankin; Univ Illinois at Chicago, Chicago, II.
- WP 028 Quantification and Proteotyping of α-1-Antitrypsin Deficiency by a Peptide MRM Assay; Linda M Benson; Yuhong Chen; Melissa R. Snyder; Jerry A. Katzmann; H. Robert Bergen, III; Mayo Clinic, Rochester, MN
- WP 029 **Dynamic Changes in the Proteome of the Postnatally Developing Mouse Brain: A Combination of 2-D DIGE and Isobaric Mass Tagging**; Babs Van de Plas<sup>1</sup>;
  Martijn Pinkse<sup>2</sup>; Gert Van den Bergh<sup>1</sup>; Stefan Clerens<sup>1,3</sup>;
  Peter D. Verhaert<sup>2</sup>; Lutgarde Arckens<sup>1</sup>; <sup>1</sup>K.U.Leuven,
  Leuven, Belgium; <sup>2</sup>Delft University of Technology, Delft,
  Netherlands; <sup>3</sup>AgResearch, Christchurch, New Zealand
- WP 030 Proteomic Analysis of the Helicobacter pylori ArsRS regulon by DIGE/MS; John T. Loh; <u>David B. Friedman</u>; Timothy L. Cover; Vanderbilt University School of Medicine, Nashville, TN
- WP 031 Quantitative Proteomics to Identify MicroRNA
  Target Proteins in Human Neoplasias; Christopher
  Lößner; Jan Meier; Uwe Warnken; Peter Lichter; Armin
  Pscherer; Martina Schnölzer; German Cancer Research
  Center, Heidelberg, Germany
- WP 032 Identification of Biomarkers to Estrogen Exposure
  Using MCF-7/BOS Cell Line Exposed to 17βEstradiol and Phytoestrogens; Mike Collodoro;
  Pascale Lemaire; Virginie Bertrand; Rowan L. Dobson;
  Gabriel Mazzucchelli; Joelle Widart; Edwin De Pauw;
  Marie-claire Gillet; University of Liège, Liège, Belgium
- WP 033 Label-Free Proteomics with MS<sup>E</sup>: Applications to Protein Functional Biology and the Biology of Adult Stem Cells; Lewis M. Brown; Grégory Boël; Nidhi Gangadhar; Brent R. Stockwell; Stuart Firestein; John F. Hunt; Columbia University, New York, NY

WP 034 Comprehensive Overview on Hyperosmotic Conditions in Corynebacterium Glutamicum;
Benjamin Fränzel; Dirk Wolters; University Bochum, Bochum, Germany

### **BIOINFORMATICS, 035 - 064**

- WP 035 **Babel Fish: Interconversion of MS File Formats and Standards**; Paul Gershon<sup>1</sup>; Panagiotis T. Papoulias<sup>2</sup>; <u>Bryan Smith</u><sup>2</sup>; Philip Andrews<sup>2</sup>; <sup>1</sup>UC-Irvine, Irvine, CA; <sup>2</sup>University of Michigan, Ann Arbor, Michigan
- WP 036 New Functionality for the Trans-Proteomic Pipeline:

  Tools for the Analysis of Proteomics Data; Luis

  Mendoza<sup>1</sup>; David Shteynberg<sup>1</sup>; Natalie Tasman<sup>1</sup>; Brian S

  Pratt<sup>2</sup>; Jimmy K. Eng<sup>3</sup>; Henry H. Lam<sup>4</sup>; Alexey

  Nesvizhskii<sup>5</sup>; Eric W. Deutsch<sup>1</sup>; Ruedi Aebersold<sup>1,6</sup>;

  <sup>1</sup>Institute for Systems Biology, Seattle, WA; <sup>2</sup>Insilicos

  LLC, Seattle, WA; <sup>3</sup>University of Washington, Seattle,

  WA; <sup>4</sup>Hong Kong University of Science and Technology,

  Clear Water Bay, Hong Kong; <sup>5</sup>University of Michigan,

  Ann Arbor, MI; <sup>6</sup>Swiss Federal Institute of Technology,

  Zurich, Switzerland
- WP 037 **Peptidome: NCBI Peptide Data Resource**; <u>Douglas J. Slotta</u>; Tanya Barrett; Ron Edgar; *NIH/NLM/NCBI*, *Bethesda*,
- WP 038 Annotation and Project Management Resource Integrated with the ProteomeCommons.org Tranche Repository; James Hill<sup>1</sup>; Bryan Smith<sup>1</sup>; Mark Gjukich<sup>1</sup>; Panagiotis G Papoulias<sup>1</sup>; Jayson Falkner<sup>2</sup>; Philip Andrews<sup>1</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI; <sup>2</sup>SOSI, Portland, OR
- WP 039 **Custom Mass-Informatics Algorithms and Workflows with MultiplierZ**; Manor Askenazi<sup>1,2</sup>;

  Jignesh Parikh<sup>2</sup>; Shaojuan Li<sup>2</sup>; Jarrod Marto<sup>2</sup>; Hebrew
  University, Jerusalem, Israel; Dana-Farber Cancer
  Institute, Boston, MA
- WP 040 Yale Protein Expression Database (YPED) Tools to Support Targeted Proteomic Analysis; Christopher
  Colangelo; Tom Abbott; Mark Shifman; Yale University, New Haven. CT
- WP 041 Scalable Cyberinfrastructure for Proteomics
  Research; Claudiu Farcas; To-Ju Huang; Roy Liu;
  Vineet Bafna; Ingolf Krueger; Pavel Pevzner; Nuno
  Bandeira; University of California, San Diego, La Jolla,
  CA
- WP 042 **DAMAGE Boosting Peptide MSMS Identification**Computing Times Using Nvidia Graphic Cards with
  a GPGPU Engine; Ivan Topolsky<sup>1</sup>; Olivier Evalet<sup>2</sup>;
  Jacques Colinge<sup>3</sup>; Anne Niknejad<sup>2</sup>; <u>Pierre-Alain Binz</u><sup>2,4</sup>;
  Alexandre Masselot<sup>2</sup>; <u>IGeneva University, Geneva,</u>
  Switzerland; <u>IGeneva Bioinformatics</u> (GeneBio),
  Geneva, Switzerland; <u>ICEMM</u>, Vienna, Austria; <u>ISWiss Institute of Bioinformatics</u>, Geneva, Switzerland
- WP 043 Using Peptide and Spectrum Indexing To Speed Up
  Mass Spectrometry Based Protein Identification; You
  Li; Leheng Wang; Hao Chi; Haipeng Wang; Yan Fu;
  Zuofei Yuan; Ruixiang Sun; Simin He; Institute of
  Computing Technology and Key Lab of I, Beijing, china,
  China
- WP 044 Analytical System of LC/MS Proteomics Data and Application; Xinjian Yan; Dmitrii Tchekhovskoi; Bhaskar Godugu; Stephen E. Stein; NIST, Gaithersburg, MD
- WP 045 Integrated Informatics Solution for Streamlining Biopharmaceutical Data Management and Reporting; Fredrick W. Schmidt; Chris L Stumpf; Waters Corporation, Milford, MA

- WP 046 Improving the Sensitivity of Peptide Identification from TandemMass Spectra using Meta-Search, Grid-Computing, and Machine-Learning; Nathan J. Edwards; Georgetown University Medical Center, Wasington, DC
- WP 047 SPIRE: Systematic Protein Identification and Relative Expression Analysis Resource for High-Throughput Proteomics; Roger Higdon<sup>1</sup>; Gregory Hather<sup>1</sup>; Andrew T Bauman<sup>1</sup>; Brent Louie<sup>1</sup>; Bill Broomall<sup>1</sup>; Simon Fortenly<sup>1</sup>; Natali Kolker<sup>1</sup>; Gerald van Belle<sup>2</sup>; Eugene Kolker<sup>1</sup>; Seattle Children's Research Institute, Seattle, WA; University of Washington, Seattle, WA
- WP 048 **High-Throughput Autonomous Proteomic Pipeline**; <u>Kebing Yu</u>; Arthur Salomon; *Brown University*, <u>Providence</u>, RI
- WP 049 STRAP: Open-Source Software for Protein
  Annotation and Data Visualization; Vivek N. Bhatia;
  David H. Perlman; Catherine E. Costello; Mark E.
  McComb; Boston University School of Medicine,
  Boston, MA
- WP 050 A New Comprehensive Software Tool for Proteomics
  Data Generated by Less Specific Enzymes; Malte
  Schürken; Michael Karas; JW Goethe Univ. of Frankf,
  Frankfurt Am Main, Germany
- WP 051 Invigorating the Mass Spectrometer: Software
  Solution for Tandem MS; Anuj Shah; Andrei Liyu;
  Yan Shi; Navdeep Jaitly; Ashoka D. Polpitiya; Joshua
  Adkins; Adam Wynne; Mikhail Belov; Ian Gorton;
  Gordon Anderson; Richard D. Smith; Pacific Northwest
  National Laboratory, West Richland, WA
- WP 052 IDSieve: An Automated Algorithm for Peptide pI Filtering of MS/MS Data to Lower False Positive and False Negative Identifications; Nikhil Garge; Benjamin J. Cargile; Jonathan L. Bundy; Maureen K. Bunger; James L. Stephenson Jr; Research Triangle Institute, Durham, NC
- WP 053 Computational MS/MS Spectra Preprocessing a Free Lunch; Bernhard Y. Renard<sup>1,2</sup>; Flavio Monigatti<sup>3</sup>; Marc Kirchner<sup>1,3</sup>; Alexander R. Ivanov<sup>4</sup>; Juri Rappsilber<sup>5</sup>; Judith A. J. Steen<sup>3</sup>; Fred A. Hamprecht<sup>1,2</sup>; Hanno Steen<sup>3</sup>; <sup>1</sup>University of Heidelberg, Heidelberg, Germany; <sup>2</sup>Children's Hospital Boston, Boston, MA; <sup>3</sup>Harvard Medical School/Children's Hospital Boston, Boston, MA; <sup>4</sup>Harvard University HSPH, Boston, MA; <sup>5</sup>Wellcome Trust Centre for Cell Biology, Edinburgh, UK
- WP 054 Consolidated Statistical Approach to Identify Cancer Biomarkers in Humoral Immune Response Study;
  Huy Vuong; Evelyn H. Kim; Chen Li; Tasneem Patwa;
  Manoj Pal; Mack Ruffin; Diane M. Simeone; David M. Lubman; University of Michigan, Ann Arbor, MI
- WP 055 Evaluation of Clustering Algorithms for Protein Complex and Protein Interaction Network Assembly;

  Mihaela Sardiu; Laurence Florens; Michael Washburn;

  Stowers Institute for Medical Research, Kansas City,

  MO
- WP 056 Express Biological Pathway Analysis of Mass
  Spectrometry Based Proteomics Datasets; Alexandre
  Podtelejnikov; Christian Ravnsborg Ingrell; Morten
  Bern; Ole Vorm; Proxeon A/S, Odense, Denmark
- WP 057 **Development of Methods and Tools for Performing**Protein Set Expression Analysis (PSEA); Roger

  Higdon<sup>1</sup>; Gregory Hather<sup>1</sup>; Andrew T Bauman<sup>1</sup>; Brent

  Louie<sup>1</sup>; Gerald van Belle<sup>2</sup>; Simon Fortenly<sup>1</sup>; Natali

  Kolker<sup>1</sup>; Bill Broomall<sup>1</sup>; Eugene Kolker<sup>1</sup>; <sup>1</sup>Seattle

- Children's Research Institute, Seattle, WA; <sup>2</sup>University of Washington, Seattle, WA
- WP 058 Molecular Networks Derived from Proteomic
  Analysis of Oral Epithelial Cells from HIV Patients
  Show High Correspondence with Known HIVInteracting Proteins; Gaurav S.J.B. Rana; Elizabeth H
  Yohannes; Santosh Gosh; Bin Jiang; Thomas
  McCormick; Aaron Weinberg; Mark Chance; Case
  Western Reserve Univers. Cleveland, OH
- WP 059 Simultaneous Multiple Alignment for LC/MS Peak Lists; Bjoern Voss¹; Bernhard Y. Renard¹; Anna Kreshuk¹; Michael Hanselmann¹; Ullrich Koethe¹; Hanno Steen²; Judith A. J. Steen²; Marc Kirchner¹,³; Fred A. Hamprecht¹; ¹University of Heidelberg, Heidelberg, Germany; ²Harvard Medical School/Children's Hospital Boston, Boston, MA; ³Children's Hospital Boston / Harvard Medical, Boston, MA
- WP 060 A Peak Alignment Algorithm for Two-Dimensional Gas Chromatography/Time-of-Flight Mass Spectrometry Based Metabolomics; Bing Wang<sup>1,2</sup>; Aiqin Fang<sup>1</sup>; Charles Buck<sup>3</sup>; Xiaodong Huang<sup>3</sup>; Xiang Zhang<sup>1</sup>; <sup>1</sup>University of Louisville, Louisville, KY; <sup>2</sup>Anhui University of Technology, Ma An Shan, China; <sup>3</sup>Purdue University, West Lafayette, IN
- WP 061 Improving Untargeted Differential Analysis of Mass Spectrometric Data by Recursive Feature Extraction; Norton Kitagawa; Steven M. Fischer; Theodore Sana; David Peterson; Ed Darland; Xiangdong Li; Agilent Technologies, Inc., Santa Clara, CA
- WP 062 Noise Analysis on Liquid Chromatography Mass Spectrometry Data on Elution Time Profile Dimension; Elias Gonzalez; Michelle Zhang; Universiyt of Texas at San Antonio, Universal City, TX
- WP 063 The Comparison of Peak-Detection Algorithms for LC/MS; Jian Cui<sup>1</sup>; gonzalez Elias<sup>1</sup>; William Haskins<sup>2</sup>; Huang Huang<sup>1</sup>; Jianqiu Zhang<sup>1</sup>; <sup>1</sup>Dept. of ECE, University of Texas at San Antonio, San Antonio, TX; <sup>2</sup>University of Texas, San Antonio, TX
- WP 064 Robust Statistical Reconstruction of Protein Profiles in Mass Spectrometry; Pierre P. Grangeat<sup>1</sup>; Grégory Strubel<sup>1</sup>; Jean-François Giovannelli<sup>2</sup>; Virginie Brun<sup>3</sup>; Laurent Gerfault<sup>1</sup>; Caroline Paulus<sup>1</sup>; Alain Dupuis<sup>3</sup>; Jérôme Garin<sup>3</sup>; ICEA, LETI, MINATEC, Grenoble, France; Université de Bordeaux, IMS/LAPS, Talence, France; CEA, INSERM, UJF, U880, iRTSV, Grenoble,

# PROTEOMICS: BIOMARKER DISCOVERY, 065 - 095

- WP 065 **Testing for Differences between Complex Samples in Proteomics Datasets**; Brian C. Searle<sup>1</sup>; David Tabb<sup>2</sup>;

  Jayson A. Falkner<sup>3</sup>; Jeffrey A. Kowalak<sup>4</sup>; Karen Meyerarendt<sup>5</sup>; Lennart Martens<sup>6</sup>; Manor Askenazi<sup>7</sup>; Paul Rudnick<sup>8</sup>; Sean L. Seymour<sup>9</sup>; William S. Lane<sup>10</sup>;

  <sup>1</sup>Proteome Software Inc., Portland, OR; <sup>2</sup>Vanderbilt University, Nashville, TN; <sup>3</sup>Single Organism Software Inc, Beaverton, Or, OR; <sup>4</sup>NIH, Bethesda, MD;

  <sup>5</sup>University of Colorado, Boulder, CO; <sup>6</sup>European Bioinformatics Institute, Cambridge, UK; <sup>7</sup>Dana-Farber Cancer Institute and Hebrew University, Boston, MA;

  <sup>8</sup>NIST, Gaithersburg, MD; <sup>9</sup>Applied Biosystems, Foster City, CA; <sup>10</sup>Harvard University, Cambridge, MA
- WP 066 Identification of Intracellular Modified Proteins by the Lipid Peroxidation Aldehyde DODE; Peter G. Slade; Michelle Williams; Viral Brahmbhtt; John S. Wishnok; Steve Tannenbaum; Massachusetts Institute of Technology, Cambridge, MA

- WP 068 Withdrawn
  WP 068 Identification of Candidate Biomarkers from
  Integrated Proteomic Analysis of Human Cancer
  Cells and Plasma from an Ovarian Cancer Mouse
  Model; Sharon J. Pitteri¹; Lellean JeBailey²; Vitor M.
  Faca¹; Melissa A. Silva¹; Renee C. Ireton¹; Jason D.
  Thorpe¹; Marc B. Horton²; Hong Wang¹; Liese Pruitt²;
  Qing Zhang¹; Kuang H. Cheng²; Nicole Urban¹; Daniela
  M. Dinulescu²; Samir M. Hanash¹; \*IFred Hutchinson
  Cancer Research Center, Seattle, WA; \*2Harvard
  Medical School, Boston, MA
  WP 069 Artifact-Free Quantitation of Free and Protein-
- WP 069 Artifact-Free Quantitation of Free and Protein-Bound Nitrotyrosine and Chlorotyrosine in Human Serum by NICI GC/MS; Yu Zeng; Kari E. Schlicht; Viral Brahmbhatt; Peter G. Slade; Lizz Liffrig; John S. Wishnok; Steven R. Tennenbaum; MIT, Cambridge, MA
- WP 070 Comparison Of Label-Free, <sup>18</sup>O/<sup>16</sup>O And Glycopeptide Enrichment For Differential Proteomics Analysis Of Human Plasma After Branched-Chain Amino Acid Infusion; Kenneth L. Johnson<sup>1,2</sup>; Carrie Holtz-Heppelmann<sup>1,2</sup>; Cristine Charlesworth<sup>1,2</sup>; Michael W. Holmes<sup>1,2</sup>; Jeanette Eckel-Passow<sup>1,3</sup>; Terry Therneau<sup>1,3</sup>; K Sreekumaran Nair<sup>1,4</sup>; H. Robert Bergen, III<sup>1,2</sup>; <sup>1</sup>Mayo Clinic, Rochester, MN; <sup>2</sup>Mayo Proteomics Research Center, Rochester, MN; <sup>3</sup>Division of Biomedical Statistics and Informatics, Rochester, MN; <sup>4</sup>Endocrinology, Rochester, MN
- WP 071 Mass Spectrometry-Based Analysis of Cerebrospinal Fluid Peptidome and Proteome for Biomarker Discovery in Alexander Disease; Robert Cunningham<sup>1</sup>; Xin Wei<sup>2</sup>; Paige Jany<sup>3</sup>; Albee Messing<sup>3</sup>; Lingjun Li<sup>4</sup>; 

  <sup>1</sup>Univ. of Wisconsin-Maidson, Madison, WI, <sup>2</sup>Univ. of Wisconsin-Madison, Madison, WI; <sup>3</sup>Waisman Center, University of Wisconsin-Madison, Madison, WI; 

  <sup>4</sup>University of Wisconsin, Madison, WI
- WP 072 Proteomic Analysis of Gynecological Mucus Samples Provides Insight into the Early Detection of Endometrial Cancer; Guangyu Zhang<sup>1</sup>; Michael Finan<sup>1</sup>; Rodney Rocconi<sup>1</sup>; Madhuri Mulekar<sup>2</sup>; Lewis K. Pannell<sup>1</sup>; <sup>1</sup>Mitchell Cancer Institute, Mobile, AL; <sup>2</sup>University of South Alabama, Mobile, AL
- WP 073 Murine Colorectal Tumor Tissue Analysis by 2D-LC/MS/MS; Wenhong Zhu; *The Burnham Institute, La Jolla, CA*
- WP 074 Discovery of Mitochondrial Protein and Phosphoprotein Biomarkers of Atrial Fibrillation;

  Mark M. Ross¹; Maryam Goudarzi¹; Weidong Zhou¹;

  Amy VanMeter¹; Lance Liotta¹; Emanuel Petricoin¹;

  Lisa Martin²; Niv Ad²; ¹George Mason University,

  Manassas, VA; ²Inova Heart & Vascular Institute, Falls

  Church, VA
- WP 075 Quantitative and Qualitative Analysis of Urinary Biomarkers by Selected Reaction Monitoring;

  Nathalie Selevsek<sup>1</sup>; Mariette Matondo<sup>1</sup>; Marta Sánchez-Carbayo<sup>2</sup>; Ruedi Aebersold<sup>1</sup>; Bruno Domon<sup>1</sup>; IETH Zurich, Zurich, Switzerland; Centro Nacional de Investigaciones Oncológicas, Madrid, Spain
- WP 076 **Proteomics Analysis of Stem Cell Secretome**; <u>Hsin-Chieh Wu</u><sup>1</sup>; Ming-Hui Yang<sup>2</sup>; Shiang-Bin Jong<sup>1</sup>; Yu-Chang Tyan<sup>1</sup>; <sup>1</sup>Kaohsiung Medical University, Kaohsiung, Taiwan; <sup>2</sup>National Sun Yat-sen University, Kaohsiung, Taiwan
- WP 077 **Identification of Glycoprotein Biomarkers in Prostate Cancer by Quantitative Proteomics**; <u>Vivekananda</u>
  <u>Shetty</u>; Thamby Gomathinayagam; Punit Shah; Zacharie

- Nickens; Ramila Philip; *Immunotope, Inc., Doylestown,* P4
- WP 078 A Quantitative Proteomic Approach for the Discovery of Prion Disease Biomarkers; Xin Wei; Allen Herbst; Judd Aiken; Lingjun Li; Univ.of Wisconsin-Madison, Madison, WI
- WP 079 Identification of Amyloid Beta Peptides in Cerebrospinal Fluid Using Isotope Dilution Liquid Chromatography and Electrospray Ionization
  Tandem Mass Spectrometry; Alfred N. Fonteh<sup>1</sup>;
  Rachel D. Fisher<sup>1</sup>; John Rush<sup>2</sup>; Michael G. Harrington<sup>1</sup>;

  \*\*IHuntington Med. Res. Insts., Pasadena, CA; \*\*2Cell Signaling Technology, Beverly, MA\*\*
- WP 080 SILAC-Labeled Cell/Tissue Lysates as a Generic Source of Proteotypic Peptides in Multiple Reaction Monitoring Analyses; Stephan Jung<sup>1</sup>; Stuart Pengelley<sup>1</sup>; Karsten Krug<sup>1</sup>; Ana Velic<sup>2</sup>; Boris Macek<sup>1</sup>; <sup>1</sup>Proteome Center Tubingen, Tubingen, Germany; <sup>2</sup>Max-Planck Institute for Biochemistry, Martinsried, Germany
- WP 081 Proteomic analysis of Sera from Prostate Cancer Patients with MALDI-TOF-MS; Corinna Henkel<sup>1</sup>; Joachim Grosse<sup>2</sup>; Gerhard Jakse<sup>2</sup>; Nadine Reulen<sup>1</sup>; Axel Heidenreich<sup>2</sup>; Ruth Knuechel<sup>1</sup>; Kristina Schwamborn<sup>1,3</sup>; 

  <sup>1</sup>Pathology, RWTH Aachen University Hospital, Aachen, Germany; <sup>2</sup>Urology, RWTH Aachen University Hospital, Aachen, Germany; <sup>3</sup>Mass Spectrometry Research Center, Biochemistry, Nashville, TN
- WP 082 Comprehensive Proteomics Analysis of Human Placental BeWo Cell Model for Preterm Birth Biomarker Discovery; Vineet Sangar<sup>1</sup>; Sumit Shah<sup>1</sup>; Samuel I Parry<sup>1</sup>; Ian A. Blair<sup>2</sup>; <sup>1</sup>University of Pennsylvania, Philadelphia, PA; <sup>2</sup>Univ. of Penn/SOM/Pharmacol, Philadelphia, PA
- WP 083 A Quantitative Proteomics Method for the Measurement of Immune Responses in HIV Resistant Women; Derek R Stein<sup>1</sup>; Terry B Ball<sup>1,2</sup>; Garrett Westmacott<sup>2</sup>; Keding Cheng<sup>2</sup>; Francis A Plummer<sup>2</sup>; 

  <sup>1</sup>University of Manitoba, Winnipeg, Canada; <sup>2</sup>Public Health Agency of Canada, Winnipeg, Canada
- WP 084 Identification of Biomarkers in Cochlear
  Pathogenesis in the Usher Syndrome 1F Mouse
  Model; Giridharan Gokulrangan<sup>1</sup>; Daniel Chen<sup>2</sup>; Sunitha
  Shyam<sup>1</sup>; Rebecca Levinson<sup>1</sup>; Nam Kim<sup>2</sup>; Mark Chance<sup>1</sup>;
  Kumar Alagramam<sup>2</sup>; <sup>1</sup>Case Center for Proteomics,
  Cleveland, OH; <sup>2</sup>Otolaryngology, Case Western Reserve
  University, Cleveland, OH
- WP 085 **Identification of Tumor-Specific Proteins in Plasma**; Yuan Tian<sup>1</sup>; Karen S. Kelly-Spratt<sup>2</sup>; Christopher J. Kemp<sup>2</sup>; Hui Zhang<sup>1</sup>; <sup>1</sup>Johns Hopkins University, Baltimore, MD; <sup>2</sup>Fred Hutchinson Cancer Research Center, Seattle, WA
- WP 086 Elucidation of Potential Diagnostic Biomarkers from Archival Fibrohistiocytic Tumor Tissue; Brian L.

  Hood<sup>1,2</sup>; Arash Radfar<sup>3</sup>; Adar T. Berghoff<sup>4</sup>; Mai Sun<sup>1,2</sup>; Uma Rao<sup>4</sup>; Thomas P. Conrads<sup>1,2</sup>; \*\*University of Pittsburgh, Pittsburgh, PA; \*\*The University of Pittsburgh Cancer Institute, Pittsburgh, PA; \*\*Department of Dermatopathology, Pittsburgh, PA; \*\*Department of Pathology, Pittsburgh, PA
- WP 087 Halogenated-Peptides as Internal Standards (H-PINS) for Liquid Chromatography Mass

  Spectrometry; Hamid Mirzaei<sup>1</sup>; Mi-Youn Bruisnak<sup>1</sup>;
  Lukas N. Mueller<sup>1</sup>; Simon Letarte<sup>1</sup>; Julian D Watts<sup>1</sup>;
  Ruedi Aebersold<sup>1,2</sup>; Institute for Systems Biology,
  Seattle, WA; Institute of Molecular Systems Biology,
  ETH Zurich, Switzerland

| WP 088 | Comparison of High Abundance Protein Depletion  |
|--------|---|
|        | Techniquesfor Biomarker Discovery with Two  |
|        | Proteomics Workflows; <u>Tim Wehr</u> <sup>1</sup> ; Chengjun Sun <sup>1</sup> ;                          |
|        | Lei Li <sup>1</sup> ; Steve Freeby <sup>1</sup> ; Ning Liu <sup>1</sup> ; John Walker <sup>1</sup> ; Aran |
|        | Paulus <sup>1</sup> ; Katrina Academia <sup>1</sup> ; Chris Sutton <sup>2</sup> ; <sup>1</sup> Bio-Rad    |
|        | Labs, Hercules, CA; <sup>2</sup> University of Bradford, Bradford,  |
|        | UK  |
|        |   |

- WP 089 Use of Pre-Spotted ProteinChip Arrays for Qualification of a MALDI TOF-TOF Instrument in Linear, Reflectron, and MS/MS Modes; Diane Mccarthy; Vanitha Thulasiraman; Amanda Bulman; Enrique Dalmasso; Fiona Plows; Bio-Rad Laboratories, Inc., Hercules, CA
- WP 090 Oxythiamine Specifically Inhibits Heat Shock Protein 27 (Hsp27) Phosphorylation and Cell Proliferation in MIA Pancreatic Cancer Cells; Rui Cao<sup>1</sup>; Hengwei Zhang<sup>1</sup>; W. Paul Lee<sup>2</sup>; Caishu Deng<sup>1</sup>; Yingchun Zhao<sup>1</sup>; Qingmei Xie<sup>1</sup>; Joan Lappe<sup>1</sup>; Robert Recker<sup>1</sup>; Songping Liang<sup>3</sup>; Gary Guishan Xiao<sup>1</sup>; Creighton University, Omaha, NE; Harbor UCLA Medical Center, Torrance, CA; College of Life Science, Hunan Normal University, Changsha, China
- WP 091 Diagnostic Feature Detection in 2-200 kDa TOF-MS
  Spectra of Leukemia Serum Proteins; Maureen B.
  Tracy; Dariya Malyarenko; Karl W. Kuschner; Eugene
  R. Tracy; William E. Cooke; Dennis Manos; College of
  William and Mary, Williamsburg, VA
- WP 092 **Proteomic Analysis of Interstitial Fluid from Head and Neck Tumors**; <u>Matthew Stone</u>; Rick M Odland; Tim Griffin; <u>University of Minnesota</u>, <u>Minneapolis</u>, <u>MN</u>
- WP 093 Discovery of Protein Markers for Lung Cancer by Label Free Mass Spectrometry and Validation in Serum; Jenny L. Heidbrink<sup>1</sup>; Tao He<sup>2</sup>; Aiqun Li<sup>1</sup>; Yeoun Jin Kim<sup>3</sup>; William FitzHugh<sup>4</sup>; Elizabeth Joseloff<sup>5</sup>; Gulshan Dhariwal<sup>1</sup>; Sudeepta Aggarwal<sup>1</sup>; Charles E. Birse<sup>1</sup>; Steven M. Ruben<sup>1</sup>; <sup>1</sup>Celera, Rockville, MD; <sup>2</sup>Wyeth, Cambridge, MA; <sup>3</sup>Bristol-Myers Squibb, Princeton, NJ; <sup>4</sup>5 AM Solutions, Reston, VA; <sup>5</sup>Cystic Fibrosis Foundation, Bethesda, MD
- WP 094 Secretome Profiling in Pancreatic Cancer Cells in Response to Transketolase Inhibitor Oxythiamine Using 15N Amino Acid Labeling and Serum-Depleted Medium; Yingchun Zhao<sup>1</sup>; Jing Xiao<sup>1</sup>; W. Paul Lee<sup>2</sup>; Rui Cao<sup>1</sup>; Robert Recker<sup>1</sup>; Vay Liang Go<sup>2</sup>; Gary Guishan Xiao<sup>1</sup>; \*\*Icreighton University, Omaha, NE; \*\*2Harbor UCLA Medical Center, Torrance, CA
- WP 095 Identification of Diagnostic Serum Biomarkers for Chagas Disease in Asymptomatic Subjects; Momar Ndao; Brian J. Ward; Christine Straccini; Bernard F. Gibbs; McGill University, Montreal, Canada

# METABOLOMICS, 096 - 130

- WP 096 Derivatization of Amino Acids in Human Plasma for Quantitation by Comprehensive Two Dimensional Gas Chromatography Time of Flight Mass Spectrometry; Elizabeth A. McGaw; Gauthier Eppe; Mark S. Lowenthal; Nathan G. Dodder; Karen W. Phinney; NIST, Gaithersburg, MD
- WP 097 High Resolution, High Accuracy Measurement and Fragmentation Analysis for Metabolite Identification in Broccoli Samples Meta-Phor Research Initiative Results; Helmut Muenster<sup>1</sup>; Eugen Damoc<sup>1</sup>; Catharina Crone<sup>1</sup>; Thomas Moehring<sup>1</sup>; Martin Hornshaw<sup>2</sup>; Madalina Oppermann<sup>1,2</sup>; Thermo Fisher Scientific (Bremen) GmbH, Bremen, GERMANY; Thermo Fisher Scientific, Hemel Hempstead, UK

- WP 098 Investigative Renal Toxicity Study in Mice Using MS-Based Metabolomics; Joanna R. Pols; Anthony Srnka; Swapan K. Chowdhury; Kevin B. Alton; Schering-Plough Research Institute, Kenilworth, NJ
- WP 099 Metal Chelating Agent Enhances Polar Anionic
  Metabolome Analysis in Nano-LC/MS; Khin Than
  Myint 1,2; Yoshiya Oda 1,2; <sup>1</sup>Eisai Co, Tsukuba, Japan;
  <sup>2</sup>CREST, Japan Science and Technology, Saitama, Japan
- WP 100 Characterizing Free Radical-Induced Indole Binding in Plasma Proteins of Huntington Disease (HD)
  Patients Using Liquid
  Chromatography/Electrochemical Array (LCECA)
  and LCMS<sup>n</sup>; Erika N. Ebbel<sup>1</sup>; Lei Wang<sup>2</sup>; Wayne R.

and LCMS"; <u>Erika N. Ebbel</u>; Lei Wang<sup>2</sup>; Wayne R. Matson<sup>3</sup>; Samantha Matson<sup>3</sup>; Swati Sharma<sup>3</sup>; Giuseppe Infusini<sup>1</sup>; Mikhail B. Bogdanov<sup>2</sup>; Steven Hersch<sup>4</sup>; Catherine E. Costello<sup>1</sup>; <sup>1</sup>Boston University School of Medicine, Boston, MA; <sup>2</sup>Weill Medical College of Cornell, New York, NY; <sup>3</sup>Bedford VA Medical Center, Bedford, MA; <sup>4</sup>Mass. General Hospital, Harvard Medical School, Charlestown, MA

- WP 101 Absolute Quantification of Amino Acids in Plasma
  Using Stable Isotope Dilution LC-MS/MS –
  Application to a Reference Material for
  Metabolomics; Mark S. Lowenthal; Gauthier Eppe;
  Elizabeth A. McGaw; Nathan G. Dodder; Karen W.
  Phinney; National Institute of Standards and
  Technology, Gaithersburg, MD
- WP 102 Characterizing Active Metabolism in Quiescent
  Human Fibroblasts; Johanna M Scarino; Hilary A
  Coller; Joshua D Rabinowitz; Aster Legesse-Miller;
  Bryson Bennett; Xiao-Jiang Feng; Princeton University,
  Princeton. NJ
- WP 103 GCxGC-TOFMS Data Interpretation of Metabolic Biomarkers from Diabetic and Nondiabetic Urine Utilizing Fisher Ratios Prior to Multivariate Analysis; John R. Heim; Scott Pugh; Mark Libardoni; LECO Corporation, St. Joseph, MI
- WP 104 Global Quantitation of Carbonyl Metabolites in Human Urine and Plasma Using <sup>12</sup>C-/<sup>13</sup>C-Dansylhydrazine Labeling and Nanolc/FT-ICR-MS;

  Margot R. Dawe; Kevin Guo; Liang Li; University of Alberta, Edmonton, Canada
- WP 105 Optimization of Mass Accuracy, Spectral Accuracy, and Resolution in Metabolite Identification Using LTQ-FT Ultra Hybrid Mass Spectrometer; Wei Zou<sup>1</sup>; Yongdong Wang<sup>2</sup>; Ming Gu<sup>2</sup>; Vladimir Tolstikov<sup>1</sup>; 

  <sup>1</sup>University of California, Genome Center, Davis, CA; 

  <sup>2</sup>Cerno Bioscience, Yardley, PA
- WP 106 Direct Single Organelle Metabolomics in a Live Single RBL-2H3 Cell by Video-Mass Spectrometry; Hajime Mizuno; Naohiro Tsuyama; Takanori Harada; Tsutomu Masujima; Hiroshima Univ. BioMed., Hiroshima, JAPAN
- WP 107 Comprehensive Analysis of Urinary Acylglycines
  Using Ultra-Performance Liquid Chromatography
  Coupled with a Hybrid Linear Ion Trap Mass
  Spectrometer; Avalyn Lewis; Liang Li; University of
  Alberta, Edmonton, Canada
- WP 108 Phosphate-Containing Metabolite Enrichment Using TiO2 and ZrO2 Microcolumns; Hyun Ju Yoo; Kristina Hakansson; University of Michigan, Ann Arbor, MI
- WP 109 A Metabolomics Study of a Breast Cancer Rat Model with Compound Identification Using an Accurate Mass Retention Time Database; Steven M. Fischer; Theodore Sana; Agilent Technologies, Santa Clara, CA

- WP 110 Biomonitoring of 2-Amino-1-Methyl-6-Phenylimidazo[4,5-b]Pyridine (PhIP) and Its Carcinogenic Metabolites in Urine; Robert J. Turesky<sup>1</sup>; Jean-Marie Fede<sup>1</sup>; Nigel J. Gooderham<sup>2</sup>; Wadsworth Center, Albany, NY; Imperial College London, London, UK
- WP 111 Uncovering the Hidden Biology of 5'Methylthioadenosine in Cancer Research Using Mass
  Spectrometry; Yibai Chen; Baiqing Tang; Warren
  Kruger; Anthony Yeung; Fox Chase Cancer Center,
  Philadelphia, PA
- WP 112 Assessing the Reproducibility of Direct Infusion Mass Spectrometric Analyses using Thermometer Ions;

  Paolo Lecchi; Jinghua Zhao; Wesley S. Wiggins; Tzong-Hao Chen; Greg P. Bertenshaw; Ping F. Yip; Brian C. Mansfield; John M. Peltier; Correlogic Systems, Inc., Rockville, MD
- WP 113 An Optimized UPLC-QTof-MS Method for Plant Metabolomics and Secondary Metabolism; David V. Huhman; Lloyd W. Sumner; The Samuel Roberts Noble Foundation, Inc., Ardmore, OK
- WP 114 Metabolomics Analysis of Saccharomyces Cerevisiae by LC/MS-TOF Using a Robust Milling Protocol for Extraction; Stefan Jenkins; Sally Webb; Theodore R. Sana; Agilent Technologies, Santa Clara, CA
- WP 115 Predicting Human Developmental Toxicity Using Human Embryonic Stem Cells and Metabolomics;
  Paul R. West; April M. Weir; Alan Smith; Sudeepa Bhattacharyya; Gabriela G. Cezar; Stemina Biomarker Discovery, Madison, WI
- WP 116 Electrospray Ionization and Collision Induced
  Dissociation of tert-Butyldimethylsilyl Derivatives of
  Endogenous Metabolites from Human Cancer Cells;
  Ruth N. Udey; Chrysoula Vasileiou; Babak Borhan; A.
  Daniel Jones; Michigan State University, East Lansing,
  MI
- WP 117 Measuring Cell to Cell Differences in the Metabolome of Individual Neurons Using Capillary Electrophoresis with Electrospray Ionization Mass Spectrometry; Theodore Lapainis<sup>1</sup>; Stanislav Rubakhin<sup>2</sup>; Jonathan V. Sweedler<sup>1</sup>; <sup>1</sup>University of Illinois, Urbana, IL; <sup>2</sup>Beckman Institute, UIUC, Urbana, II.
- WP 118 GC/APCI-TOF MS: A New Valuable Tool for Analysis of Biofluids in Metabolomics Studies; Alegria Carrasco-Pancorbo<sup>1</sup>; Ekaterina Nevedomskaya<sup>1</sup>; Tiziana Pacchiarotta<sup>1</sup>; Ali Kettani<sup>2</sup>; Thomas Arthen-Engeland<sup>3</sup>; Gabriela Zurek<sup>3</sup>; Carsten Baessmann<sup>3</sup>; Oleg Mayboroda<sup>1</sup>; Andre Deelder<sup>1</sup>; <sup>1</sup>LUMC, Leiden, NL; <sup>2</sup>Bruker Daltonics Inc., Fremont, CA; <sup>3</sup>Bruker Daltonik GmbH, 28359 Bremen, Germany
- WP 119 A Laboratory Information Management System (LIMS) for High-Throughput LC-MS Metabolomics-Based Biomarker Discovery; Alan Smith<sup>1</sup>; Yuerong Zhu<sup>2</sup>; Paul R. West<sup>1</sup>; April M. Weir<sup>1</sup>; Sudeepa Bhattacharyya<sup>1</sup>; Gabriela G. Cezar<sup>1</sup>; <sup>1</sup>Stemina Biomarker Discovery, Madison, WI; <sup>2</sup>BioInfoRx, Inc., Madison, WI
- WP 120 Challenges in the Investigation of the Metabolic Changes in Nicotiana Attenuata during Insect Herbivory Using an Improved HPLC-TOF-MS Method; Matthias Schoettner<sup>1</sup>; Beatrice Berger<sup>1</sup>; Emmanuel Gaquerel<sup>1</sup>; Eva Rothe<sup>1</sup>; Birgit Schneider<sup>2</sup>; Gabriela Zurek<sup>2</sup>; Aiko Barsch<sup>2</sup>; Mike Mcdonell<sup>3</sup>; Ian T. Baldwin<sup>1</sup>; <sup>1</sup>MPI Chemical Ecology, Jena, Germany; <sup>2</sup>Bruker Daltonik GmbH, Bremen, Germany; <sup>3</sup>Bruker Bioscience, Delta, BC

- WP 121 Identification of Metabolites in a Human Plasma
  Standard Reference Material by Comprehensive two
  Dimensional Gas Chromatography-Time-of-Flight
  Mass Spectrometry; Gauthier Eppe; Elizabeth A.
  McGaw; Nathan G. Dodder; Bruce A. Benner Jr; Karen
  W. Phinney; Michele M. Schantz; NIST, Gaithersburg,
  MD
- WP 122 Metabolomics-Based Approach to Antibiotic Resistance in Staphylococcus Aureus; <u>Kyu Rhee</u><sup>2</sup>; Steven M. Fischer<sup>1</sup>; Elizabeth Alexander<sup>2</sup>; <sup>1</sup>Agilent Technologies, Santa Clara, CA; <sup>2</sup>Weill Cornell Medical College, NY, NY
- WP 123 Metabolite Profiling of the Novel NIST Standard
  Human Plasma Using a Multi-Target Calibration
  Approach in GC/Quadrupole MS; Mine Palazoglu;
  Sevini Shahbaz; Oliver Fiehn; UC Davis, Davis, CA
- WP 124 Precision and Accuracy of Carbon Isotope Ratios is
  Critical for Isotopomer-Based Metabolomics: A
  Comparative study of FTICR and NMR; Bogdan
  Bogdanov<sup>1</sup>; Teresa W Fan<sup>1,2</sup>; Andrew N Lane<sup>1,2</sup>; Richard
  M Higashi<sup>1,2</sup>; <sup>1</sup>University of Louisville Department of
  Chemistry, Louisville, KY; <sup>2</sup>James Graham Brown
  Cancer Center, Louisville, KY
- WP 125 Metabolomics of Volatile Compounds by a New BinBase Mass Spectral Database; Gert Wohlgemuth; Kirsten Skogerson; Oliver Fiehn; UC Davis, Davis, CA
- WP 126 The Metabolomic Analysis of Simvastatin Dosed Rat Plasma by GC/TOF/MS; Henry Y. Shion<sup>1</sup>; John P. Shockcor<sup>1</sup>; Douglas Stevens<sup>3</sup>; Jose Castro-perez<sup>1</sup>; Kate Yu<sup>1</sup>; Emma Marsden-edwards<sup>2</sup>; Eleni Gika<sup>4</sup>; Georgios Theodoridis<sup>4</sup>; Ian Wilson<sup>5</sup>; <sup>1</sup>Waters Corp., Milford, MA; <sup>2</sup>Waters Corporation, manchester, UK; <sup>3</sup>Waters Corp, Holden, MA; <sup>4</sup>Aristotle University, Thessaloniki, Greece: <sup>5</sup>Astra Zeneca. Macclesfield. UK
- WP 127 Identification of Key Metabolic Pathways in Polycystic Ovary Syndrome by Mass Spectrometry, NMR and Cavity Ring Down Spectroscopy; Michael R. Shortreed<sup>1</sup>; Fariba Assadi-Porter<sup>1</sup>; Leah D. Whigham<sup>1</sup>; Mark E. Cook<sup>1</sup>; Butz Daniel<sup>1</sup>; Warren P. Porter<sup>1</sup>; David H. Abbott<sup>1</sup>; John L. Markley<sup>1</sup>; Hamid Eghbalnia<sup>2</sup>; Lloyd M. Smith<sup>1</sup>; \*\*University of Wisconsin, Madison, WI; \*\*2University of Cincinnati, Cincinnati, OH
- WP 128 Comparison and Combination of Direct Infusionand LC-FTMS for Comprehensive Plant Metabolomics; Jun Han<sup>1</sup>; Ryan M Danell<sup>2</sup>; Monica H Elliott<sup>1</sup>; Michael Deyholos<sup>3</sup>; Christoph H Borchers<sup>1</sup>; <sup>1</sup>UVic-GBC Proteomics Centre, Victoria, Canada; <sup>2</sup>Danell Consulting, Greenville, NC; <sup>3</sup>Dept Biological Sciences, University of Alberta, Edmonton, AB, Canada
- WP 129 Single Cell Differential Metabolomics for Stimulated Allergy Cells; Shoko Inoue; Hajime Mizuno; Naohiro Tsuyama; Takanori Harada; Tsutomu Masujima; Hiroshima Univ. BioMed., Hiroshima City, Japan
- WP 130 Biomarker Discovery in a Glaucoma Study Using Targeted and Non-Targeted Metabolomics
  Approaches; Richard Schneider<sup>1</sup>; Marielle
  Delnomdedieu<sup>1</sup>; Andy Butler<sup>1</sup>; Poulabi Banerjee<sup>1</sup>; Klaus Weinberger<sup>2</sup>; Denise Sontag<sup>2</sup>; \*\*Pfizer Global R&D, Groton, CT; \*\*PBiocrates Life Sciences, Innsbruck, Austria

# PROTEOMICS: NEW APPROACHES, 131 - 157

WP 131 Extending the Dynamic Range of Proteome
Measurement in a Natural Microbial Community
with IEF Protein Fractionation and
Multidimensional LC-MS/MS; Brian D. Dill<sup>1</sup>; Paul
Wilmes<sup>2</sup>; Vincent Denef<sup>2</sup>; Manesh Shah<sup>1</sup>; Michael P.
Thelen<sup>3</sup>; Brian Erickson<sup>1,4</sup>; Robert Hettich<sup>1</sup>; Jill F.

- Banfield<sup>2</sup>; Nathan C. VerBerkmoes<sup>1</sup>; <sup>1</sup>Oak Ridge National Laboratory, Oak Ridge, TN; <sup>2</sup>University of California, Berkeley, Berkeley, CA; <sup>3</sup>Pacific Northwest National Laboratory, West Richland, WA; <sup>4</sup>University of Tennessee, Knoxville, TN
- WP 132 Love It or Leave It... On the Use of SDS in GELFrEE for Protein Prefractionation and MS Analysis; Alan A. Doucette; Fang Liu; Dalhousie University, Halifax, Canada
- WP 133 Use of Low Conductivity Buffers in Isoelectric
  Trapping Separations and MS Analysis; Stephanie M.
  Cologna; William K. Russell; Gyula Vigh; David H.
  Russell; Texas A&M University, College Station, TX
- WP 134 Proteome Prefractionation Using Three
  Complimentary 2D Solution Phase Platforms; Mark J.
  Wall; Alan A. Doucette; Dalhousie University, Halifax,
  Canada
- WP 135 Comparison of 2-D and 3-D Protein Profiling of Melanoma Cells: Depth of Analysis and Reproducibility of Protein Detection; Huan Wang; Tony Chang-Wong; Hsin-Yao Tang; David W. Speicher; The Wistar Institute, Philadelphia, PA
- WP 136 Protein Separation and Identification Using Thin-Layer Chromatography Coupled With Electrospray-Assisted Laser Desorption Ionization Mass Spectrometry; Min-Zong Huang; Ya-Ting Chan; Jentaie Shiea; National Sun Yat-Sen Univ., Kaohsiung, Taiwan
- WP 137 Surface-Enhanced Protein Analysis: Effect of Different Surfaces on Reflectron Profiling and MS/MS Analysis Using ToF-ToF Instrumentation;

  Fiona Plows<sup>1</sup>; Vanitha Thulasiraman<sup>1</sup>; Matthew Hammond<sup>1</sup>; Steve Roth<sup>1</sup>; Mariana Rusa<sup>1</sup>; Diane McCarthy<sup>2</sup>; <sup>1</sup>Bio-Rad Laboratories, Inc., Hercules, CA; <sup>2</sup>Bio-Rad, Malvern, PA
- WP 138 Selective Purification of Azide-Containing Peptides from Complex Mixtures; Merel A. Nessen; Gertjan Kramer; JaapWillem Back; Linde E.J. Smeenk; Jan H. van Maarseveen; Leo J. de Koning; Luitzen de Jong; Henk Hiemstra; Chris G. de Koster; University of Amsterdam, Amsterdam, Netherlands
- WP 139 Analytical Liquid-Liquid Electroextraction Coupled to LC-MS to Enhance the Detection Limits of Peptides; Peter Lindenburg<sup>1</sup>; Ubbo Tjaden<sup>1</sup>; Jan Van Der Greef<sup>1,2</sup>; Thomas Hankemeier<sup>1</sup>; ILeiden University, Leiden, Netherlands; <sup>2</sup>TNO Systems Biology, Aj Zeist, Netherlands
- WP 140 Merging Single-Particle Electron Microscopy and Mass-Spectrometry-Based Proteomics EM Carbon-Film-Assisted Endoproteinase Digestion (ECAD);

  Florian M. Richter<sup>1</sup>; Monika M. Golas<sup>2</sup>; Björn Sander<sup>2</sup>;

  Berthold Kastner<sup>3</sup>; Reinhard Lührmann<sup>3</sup>; Holger Stark<sup>4</sup>;

  Henning Urlaub<sup>1</sup>; \*\*Bioanalytical MS, MPI Biophysical Chemistry, Göttingen, Germany; \*\*2EM Research Laboratory, University of Århus, Århus, Denmark;

  \*\*Cellular Biochemistry, MPI Biophysical Chemistry, Göttingen, Germany; \*\*43D Electron Microscopy, MPI Biophysical Chemistry, Göttingen, Germany
- WP 141 Novel Efficient and Automated On-Line Enrichment Strategy for Phosphopeptide Analysis; Yelena Margolin<sup>1</sup>; Bogdan A. Budnik<sup>2</sup>; Emily Freeman<sup>1</sup>; William S. Lane<sup>2</sup>; Alexander R. Ivanov<sup>1</sup>; <sup>1</sup>Harvard University, HSPH, Boston, MA; <sup>2</sup>Harvard University, Cambridge, MA
- WP 142 Dynamic Range Compression via Hexapeptide Libraries for Increased Proteome Coverage in Whole

- **Human Saliva**; <u>Sricharan Bandhakavi</u>; Matthew D Stone; Timothy J Griffin; *University of Minnesota, Minneapolis, MN*
- WP 143 Squid Neuron Analysis: Applying Proteomic
  Software Tools to LC/MS/MS Data from Species
  without Annotated Genomes; Anthony J. Makusky²;
  Joseph A. DeGiorgis¹; Jeffrey A. Kowalak²; Sanford P.
  Markey²; ¹Providence College, Providence, RI; ²NIMH,
  NIH. Bethesda. MD
- WP 144 Comparison of Proteogenomic Approaches Across Kingdoms: A Joint Effort in Gene Modeling; Samuel O. Purvine<sup>1</sup>; Kim K. Hixson<sup>1</sup>; Muktak Aklujkar<sup>2</sup>; Ellen Panisko<sup>1</sup>; Lee Ann McCue<sup>1</sup>; Matthew Monroe<sup>1</sup>; Lykidis Athanasios<sup>3</sup>; Kyrpides Nikos<sup>3</sup>; Deanna Auberry<sup>1</sup>; Derek Lovely<sup>2</sup>; Grigoriev Igor<sup>3</sup>; Scott Baker<sup>1</sup>; Mary Lipton<sup>1</sup>; Gordon Anderson<sup>1</sup>; Richard D. Smith<sup>1</sup>; <sup>1</sup>Pacific Northwest National Laboratory Battelle, Richland, WA; <sup>2</sup>University of Massachusetts, Amherst, Massachusetts; <sup>3</sup>Joint Genome Institute, Walnut Creek, California
- WP 145 Deconvolution of Isotopically Unresolved Multiply Charged States of Intact Proteins and Peptides;

  Natalia Belyaeva; Tonya Second; Thermo Fisher
  Scientific, San Jose, CA
- WP 146 Optimization of a LC-FTMS Proteomics Pipeline for High Throughput and Confident Peptide Identifications; Ronald J. Moore; Aleksey Tolmachev; Anil K. Shukla; Therese R.W. Clauss; Rui Zhang; David J. Anderson; Karl K. Weitz; Brianne O. Petritis; Richard D. Smith; Pacific Northwest National Laboratory, Richland, WA
- WP 147 A Novel Way to Observe Protein Interaction
  Environments Using the Global Proteome Machine
  Database; Chengcheng Zhang; Dan Evans; Ronald
  Beavis; Juergen Kast; University of British Columbia,
  Vancouver, Canada
- WP 148 A Comparison of Calibration Equations for Improving Mass Accuracy by Internal Recalibration of TOF MS/MS Data Sets From Whole-cell Digests;

  Cesar Costa Vera<sup>1</sup>; André M. Deelder<sup>2</sup>; Magnus Palmblad<sup>2</sup>; \*\*IEscuela Politécnica Nacional / Dept. de Física, Quito, Ecuador; \*\*2Leiden University, Leiden, Netherlands\*\*
- WP 149 Quantifying Multiplexed MS/MS Spectral
   "Chimeras" in Shotgun Proteomics; Stephane Houel;
   Robert A. Abernathy; Kutralanathan Renganatahan; Eric
   S. Witze; Chia-yu Yen; Karen Meyer-Arendt; Katheryn
   A. Resing; Natalie G. Ahn; William M. Old; Univ. of
   Colorado, Boulder, CO
- WP 150 An Information-Dependent Iterative MS/MS
  Acquisition (IMMA) Tool for Non-redundant Protein
  Identification on a LC MALDI MS/MS Platform;
  Haichuan Liu¹; Lee Yang²; Nikita Khainovski³; Simon
  Allen¹; Ming Dong²; Evelin D. Szakal¹; Megan Choi²;
  Steven Hall¹; Susan Fisher¹; Jian Jin²; H. Ewa
  Witkowska¹; Mark D. Biggin²; ¹UCSF Sandler-Moore
  Mass Spectrometry Core Facility, San Francisco, CA;
  ²Lawrence Berkeley National Laboratory, Berkeley, CA;
  ³Consultant, Framingham, MA
- WP 151 Statistical Calibration of XCorr is More Important for Spectra Derived Using Data-Independent Acquisition; Sean Mcilwain; Michael J. Maccoss; William Noble; University of Washington, Seattle, WA
- WP 152 Fast and Accurate Identification of Cross-Linked Peptides for the Structural Analysis of Large Protein Complexes and to Elucidate Interaction Networks;

- <u>Salman Tahir</u>; Jimi-Carlo Bukowski-Wills; Morten Rasmussen; Juri Rappsilber; *Wellcome Trust Centre for Cell Biology, Edinburgh, UK*
- WP 153 Development of a Mass-Spectrometry Identifiable Cross-Linker and Application to a the 34K-Actin Protein System; Lisabeth Hoffman<sup>1</sup>; Paul Griffin<sup>1</sup>; Marcus Fechheimer<sup>1</sup>; Evgeniy Petrotchenko<sup>2</sup>; Christoph Borchers<sup>2</sup>; Jon Amster<sup>1</sup>; \*\*Iuniversity of Georgia, Athens, GA: \*\*2UVic-GBC Proteomics Centre, Victoria, BC\*\*
- WP 154 Analysis of Crosslinked Proteins Using a Marker-Ion Labeled Crosslinker; Tobias Beckhaus; N. Arrey Tabiwang; Florian Durst; Volker Doetsch; Michael Karas; Goethe-University of Frankfurt, Frankfurt Am Main, Germany
- WP 155 Mapping Protein-Protein Interactions in Human Serum with the Protein Interaction Reporter (PIR)/Chemical Cross-Linking Strategy; Chad Weisbrod<sup>2</sup>; Li Yang<sup>1</sup>; Xiaoting Tang<sup>2</sup>; James Bruce<sup>2</sup>; 

  \*\*Washington State University, Pullman, WA; \*\*University of Washington, Seattle, WA\*\*
- WP 156 Novel Photo-Cleavable Protein Interaction Reporter (pcPIR) Cross-Linking and Data-Dependent MS/MS Strategy for Studying Protein-Protein Interactions;

  Li Yang¹; Xiaoting Tang²; Gerhard Munske¹; James Bruce²; ¹Washington State University, Pullman, WA;

  2 University of Washington, Seattle, WA
- WP 157 Monitoring Protein Conformation Changes as an Activating Step for Protein Interactions with Cross-Linking/MS Analysis; Zhuo Chen<sup>1</sup>; Morten Rasmussen<sup>1</sup>; Salman Tahir<sup>1</sup>; C.A.C Clark<sup>2</sup>; Paul Barlow<sup>2</sup>; Juri Rappsilber<sup>1</sup>; <sup>1</sup>Wellcome Trust Centre for Cell Biology, Edinburgh, UK; <sup>2</sup>School of Chemistry, University of Edinburgh, Edinburgh, UK

# **SMALL MOLECULE ANALYSIS, 158 - 177**

- WP 158 Top-Down Identification of Dihydroergoloids in Equine Plasma by MS<sup>n</sup> Ion Tree Mass Spectrometry and High Resolution Accurate Mass Analysis; Jeffrey Rudy<sup>1</sup>; Carisa Dixon<sup>2</sup>; Cornelius Uboh<sup>1,2</sup>; Lawrence Soma<sup>2</sup>; <sup>1</sup>PA Equine Toxicology, West Chester, PA; <sup>2</sup>University of Pennsylvania, Kennett Square, PA
- WP 159 Investigations into Drug Stability Using LC-MS-MS
  Data Combined with Statistical Analysis; Stephen
  Rumbelow<sup>1</sup>; Johnie Brown<sup>2</sup>; \*\*I Croda Inc, New Castle,
  DE; \*\*Papplied Biosystems, Framingham, MA\*\*
- WP 160 LC/MS/MS Determination of Gemcitabine
  Incorporation into DNA as a Useful Surrogate for
  Optimizing Drug Exposure; Barry R. Jones<sup>1</sup>; Barry
  Lutzke<sup>2</sup>; Enaksha R Wickremsinhe<sup>2</sup>; Bradley L.
  Ackermann<sup>2</sup>; Angela M. Bones<sup>2</sup>; Angela B. Freeman<sup>2</sup>;
  Susan E. Pratt<sup>2</sup>; Christopher A. Schmalz<sup>2</sup>; Gary A.
  Schultz<sup>1</sup>; Advion BioServices, Inc., Ithaca, NY; Eli
  Lilly & Company, Indianapolis, IN
- WP 161 Unambiguous Assignment of the Elemental
  Composition through the Use of A Fuzzy Logic
  Algorithm; Richard Gedamke<sup>1</sup>; Serhiy Hnatyshyn<sup>1,2</sup>;

  Bristol-Myers Squibb, New Brunswick, NJ; BMS Co.,
  Princeton, NJ
- WP 162 Laser Desorption Mass Spectrometric Analysis of Paints and Pigments Used by Modern Artists; Daniel P. Kirby; Narayan Khandekar; Lynn Lee; Straus Center, Harvard, Cambridge, MA
- WP 163 Gas Chromatography SALDI: Importance of Proton Affinity and Laser Fluence to Sensitivity and Ion Fragmentation; Sergey Alimpiev<sup>2</sup>; Alexander Grechnikov<sup>3</sup>; Jan Sunner<sup>1</sup>; Alexey Borodkov<sup>3</sup>; Serfey Nikiforov<sup>2</sup>; Yaroslav Simanovsky<sup>2</sup>; <sup>1</sup>University of

- Portsmouth, Portsmouth, UK; <sup>2</sup>Prokhorov General Physics Inst Russ Acad Sci, Moscow, Russia; <sup>3</sup>Vernadsky Institute Geochemisty Analytical Chem, Moscow, Russia
- WP 164 Distinguishing Regioisomers of Carboxylated Aromatic Analytes via Atmospheric Pressure Chemical Ionization and Tandem Mass

  Spectrometry; Lucas Amundson<sup>1</sup>; Steven Habicht<sup>1</sup>; Vanessa Gallardo<sup>1</sup>; Mingkun Fu<sup>1</sup>; Ryan Shea<sup>2</sup>; Allen Mossman<sup>2</sup>; Hilkka Kenttamaa<sup>3</sup>; Hilkka Kenttamaa<sup>3</sup>; 

  1 Purdue University, West Lafayette, IN; 2BP Chemicals, Naperville, IL; 3 Chemistry Department, West Lafayette, IN
- WP 165 A New Robust Library Search Algorithm for LC-MSMS of Small Molecules and its Spectral Library Sharing Mechanism; Yann Mauron<sup>1</sup>; Roman Mylonas<sup>1</sup>; Alexandre Masselot<sup>2</sup>; Pierre-Alain Binz<sup>1,2</sup>; Marc Fathi<sup>3</sup>; Veronique Viette<sup>4</sup>; Denis F Hochstrasser<sup>3,5</sup>; Frederique Lisacek<sup>1</sup>; <sup>1</sup>Swiss Institute of Bioinformatics, Geneva, Switzerland; <sup>2</sup>Geneva Bioinformatics (GeneBio), Geneva, Switzerland; <sup>3</sup>Geneva University Hospitals, Geneva, Switzerland; <sup>4</sup>ADMed Fundation, La Chaux-de-Fonds, Switzerland; <sup>5</sup>Swiss Center for Applied Humen Toxicology, Geneva, Switzerland
- WP 166 New Qualitative Screening Software for Automated Small Molecule Multi-Target Analysis; Graham A.

  McGibbon¹; Mark A. Bayliss¹; Vitaly Lashin²;

  Advanced Chemistry Development Inc., Toronto, ON;

  Advanced Chemistry Development, Ltd, Moscow,

  Russia
- WP 167 Determination of Relative Affinities of Staurosporine Derivatives for Quinone Reductase-2 Using Ultrafiltration of LC-MS; Yongsoo Choi<sup>1</sup>; Megan Sturdy<sup>1</sup>; Katherine Maloney<sup>2</sup>; Sang Jip Nam<sup>2</sup>; Shunyan Mo<sup>1</sup>; Andrew D Mesecar<sup>1</sup>; John M Pezzuto<sup>3</sup>; William Fenical<sup>2</sup>; Jimmy Orjala<sup>1</sup>; Richard B. van Breemen<sup>1</sup>; 

  <sup>1</sup>University of Illinois College of Pharmacy, Chicago, IL; <sup>2</sup>University of California, La Jolla, California; 

  <sup>3</sup>University of Hawaii at Hilo, Hilo, Hawaii
- WP 168 Live Single Cell Video-Mass Spectrometry for Straightforward Analysis of Cellular Pathways;

  Tsutomu Masujima; Naohiro Tsuyama; Hajime Mizuno; Hiroshima Univ. BioMed., Hiroshima, Japan
- WP 169 Mass Spectrometric Analysis of Small Molecules
  Using Nano-Assisted Laser Desorption/Ionization
  (NALDI) MS; Chul Yoo¹; Michael Ronk¹; David J.
  Semin¹; Sam Fu²; Joseph P. Fox²; Gongyi Shi²; ¹Amgen,
  Inc., Thousand Oaks, CA; ²Bruker Daltonics, Fremont,
- WP 170 Purity Analysis of HTS Compounds for the National Toxicology Program Utilizing Liquid
  Chromatography Mass Spectrometry; Lisa L. Haney<sup>1</sup>;
  Leslie L. Moody<sup>1</sup>; Kim T. Thornton<sup>1</sup>; Bart A. O'Brien<sup>1</sup>;
  Roger K. Harris<sup>1</sup>; Peter J. Schebler<sup>1</sup>; Joseph W. Algaier<sup>1</sup>;
  Beby Jayaram<sup>2</sup>; Cynthia S. Smith<sup>2</sup>; <sup>1</sup>Midwest Research Institute, Kansas City, MO; <sup>2</sup>National Toxicology
  Program NIEHS, Research Triangle Park, NC
- WP 171 A Sensitive LC-MS/MS Method for the Determination of KX2-391 in Human Plasma;

  Xinping Fang¹; Dawei Zhou¹; Anh Pharm¹; David, G. Hangauer²; Jinn Wu¹; ¹XenoBiotic Laboratories, Inc., Plainsboro, NJ; ²Kinex Pharmaceuticals, LLC, Buffalo, NY
- WP 172 New Algorithm for Determination of Isotopic Envelopes on Labelled Compounds, Comparison of MS and MS/MS Platforms for Isotopic Abundance

- Measurements; Gustaf Hulthe; Sofia Essén; Magnus Johansson; Medicinal Chemistry, Mölndal, Sweden
- WP 173 Monitoring Levels of Salsolinol and
  Neurotransmitters in the Brain of Alcohol Preferring
  Rats Exposed to Alcohol and Treated with
  Ceftriaxone; Youssef Sari<sup>2</sup>; Loubna A. Hammad<sup>1</sup>;
  Marwa M. Saleh<sup>1</sup>; George V. Rebec<sup>2</sup>; Yehia Mechref<sup>1</sup>;

  \*\*Department of Chemistry, Indiana University,
  Bloomington, IN; \*\*Department of Psychological, Indiana
  University, Bloomington, IN
- WP 174 Feasibility and Reliability of Low and High-Resolution MS Approaches for Accurate Mass and Molecular Formula Determination in Drug Discovery; Vladimir Capka<sup>1</sup>; Ming Gu<sup>2</sup>; <sup>1</sup>Astra Zeneca R&D Boston, Waltham, MA; <sup>2</sup>Cerno Bioscience, Yardley, PA
- WP 175 Optimizing Mass Spectrometric Detection for Ion Chromatography: I. Common Anions and Organic Acids; Jinyuan Wang; Stacy Henday; William C. Schnute; Dionex Corporation, Sunnyvale, CA
- WP 176 Investigation of Infrared Multiphoton Dissociation with Potential Application to Pharmaceutically-Relevant Compounds; K Wayne Taylor; Lilly, Indianapolis, IN
- WP 177 Mass Spectral Method for the Quantification of Host-Guest Interactions Including Ionophore-Siderophore Assemblies; Esther M. Tristani; George R. Dubay; Alvin L. Crumbliss; Duke University, Durham, NC

# **IMAGING MS: PEPTIDES AND PROTEINS, 178 - 195**

- WP 178 Spatially-Resolved Proteomic Analysis of Chick Heart Valves; Andrew K. Gelasco<sup>1</sup>; Angus C. Grey<sup>2</sup>; Ricardo A. Moreno-Rodriguez<sup>1</sup>; Edward L. Krug<sup>1</sup>; Kevin L. Schey<sup>2</sup>; \*\*Image of South Carolina, Charleston, SC; \*\*2Vanderbilt University, Nashville, TN
- WP 179 MALDI Imaging of Prostate Cancer Tissue Toward Validation of Biomarker Identification; Christopher Hattan<sup>1</sup>; Barbara Leinweber<sup>1</sup>; Raymond Nagle<sup>2</sup>; Jaime Gard<sup>2</sup>; Gary Pestano<sup>3</sup>; Phillip Miller<sup>3</sup>; Jan Froehlich<sup>3</sup>; Gongyi Shi<sup>4</sup>; Gary Kruppa<sup>4</sup>; George Tsaprailis<sup>5</sup>; Serrine S. Lau<sup>1</sup>; <sup>1</sup>Univ of Arizona, Pharmacy, Tucson, AZ, <sup>2</sup>Univ of Arizona, Medicine, Tucson, AZ, <sup>3</sup>Ventana Medical Systems, Tucson, AZ; <sup>4</sup>Bruker Daltonics, Billerica, MA; <sup>5</sup>Center for Toxicology, Tucson, AZ
- WP 180 Mapping VEGF Splice Variants in the Rat Model of Retinopathy by MALDI IMS; <u>Joey C. Latham</u>; Susan E. Yanni; John S. Penn; Richard M. Caprioli; *Vanderbilt Univ Sch of Med, Nashville, TN*
- WP 181 Imaging Therapeutic "Decoy" Oligodeoxynucleotide within Tissue Sections by MALDI MS; Rita Casadonte<sup>1</sup>; Joseph M. Amann<sup>1</sup>; Jennifer R. Grandis<sup>2</sup>; David P. Carbone<sup>1</sup>; Richard M. Caprioli<sup>1</sup>; \*Vanderbilt Univ Sch of Med, Nashville, TN; \*2University of Pittsburgh School of Medicine, Pittsburgh, Pennsylvania
- WP 182 MALDI Mass Spectrometric Imaging of Nervous Tissue Using the Stretched Sample Method; Tyler A Zimmerman<sup>1</sup>; Stanislav Rubakhin<sup>2</sup>; Elena Romanova<sup>1</sup>; Jonathan Sweedler<sup>1</sup>; <sup>1</sup>University of Illinois, Urbana, IL; <sup>2</sup>Beckman Institute, UIUC, Urbana, IL
- WP 183 Utilizing NIMS and MALDI Imaging Mass
  Spectrometric Techniques for Lipidomic and
  Peptidomic Studies of Crab and Murine Brain;
  Robert Sturm<sup>1</sup>; Ruibing Chen<sup>1</sup>; Hin-Koon Woo<sup>2</sup>; Oscar
  Yanes<sup>2</sup>; Gary Siuzdak<sup>2</sup>; Lingjun Li<sup>1</sup>; <sup>1</sup>University of
  Wisconson-Madison, Madison, WI; <sup>2</sup>The Scripps
  Research Institute, La Jolla, CA

- WP 184 Imaging Mass Spectrometry Reveals Peptide
  Partitioning in MALDI Samples; Delphine Debois;
  Pascale Lemaire; Loic Quinton; Valerie Gabelica; Edwin
  De Pauw; University of Liege, LSM-CART, Liège,
  Belgium
- WP 185 Visualization of Mouse Cardiovascular Modeling from Embryonic Day 14.5 to Adult by High Resolution MALDI Imaging; Peggi Angel<sup>1</sup>; Pierre Chaurand<sup>1</sup>; Joey V. Barnett<sup>1,2</sup>; H. Scott Baldwin<sup>1,2</sup>; Richard M. Caprioli<sup>2</sup>; <sup>1</sup>Vanderbilt University Medical Center, Nashville, Tennessee; <sup>2</sup>Vanderbilt Univ Sch of Med, Nashville, TN
- WP 186 Comparison of Laser Desorption 7.87 eV
  Postionization Mass Spectrometry with MALDI for
  Detection of Peptides in Bacterial Biofilms; Artem
  Akhmetov<sup>1</sup>; Gerald Gasper<sup>1</sup>; Chhavi Bhardwaj<sup>1</sup>; Peter
  Koin<sup>1</sup>; Ross Carlson<sup>2</sup>; Jerry F. Moore<sup>3</sup>; Luke Hanley<sup>1</sup>;

  <sup>1</sup>University Illinois Chicago, Chicago, IL; <sup>2</sup>Montana
  State University, Bozeman, MT; <sup>3</sup>MassThink LLC,
  Naperville, IL
- WP 187 Analysis of Potential Biomarkers in Human Ovarian Cancer Using MALDI Imaging Mass Spectrometry;

  Yanfeng Chen; Ying Liu; Rebecca Shaner; DeEtte
  Walker; John McDonald; Alfred Merrill; Mark Cameron Sullards; Georgia Institute of Technology, Atlanta, GA
- WP 188 MALDI Imaging of Posttranslationally Modified Proteins; Kevin L. Schey; Angus Grey; Vanderbilt University, Nashville, TN
- WP 189 Isobaric Mass Tags for Quantitative Multiplexed Imaging of mRNA Distributions by in-situ Hybridisation and MALDI-MS; Emrys A Jones<sup>1</sup>; Adam McMahon<sup>1</sup>; Andrew Thompson<sup>2</sup>; Emmanuel Raptakis<sup>3</sup>; <sup>1</sup>University of Manchester, Manchester, UK; <sup>2</sup>Trillion Genomics, Cambridge, UK; <sup>3</sup>Kratos Analytical, Manchester, UK
- WP 190 Multiple Sequential Imaging of PL's, Proteins, and Peptides on a Single Tissue Section using MALDI IMS; William Hardesty<sup>1</sup>; Richard M. Caprioli<sup>2</sup>; 

  Vanderbilt University, Nashville, TN; <sup>2</sup>Vanderbilt Univ Sch of Med, Nashville, TN
- WP 191 Imaging Mass Spectrometry Comparative Analysis of Human Pancreatic Adenocarcinoma, Insulinoma and Control; Alexandra van Remoortere; René J.M. van Zeijl; Stefan M. Willems; André M. Deelder; Liam Mcdonnell; LUMC, Leiden, Netherlands
- WP 192 Chemical Molecular Imaging for Nanoparticles
  Induced Brain and Lung Damage Animal Models by
  MALDI-TOF MS; Jen-kun Chen; Yi-Ting Wu; JuiPing Li; Chia-Hua Chen; Chung-Shi Yang; National
  Health Research Institutes, Zhunan, Taiwan
- WP 193 FT-ICR and SIMS-TOF Imaging Mass Spectrometry for the Characterization of Human Pancreatic Disease; Donald F. Smith<sup>1</sup>; Marc C. Duursma<sup>1</sup>; Michael Hanselmann<sup>2</sup>; Fred A. Hamprecht<sup>2</sup>; Nathalia A. Giese<sup>2</sup>; Ron M.A. Heeren<sup>1</sup>; <sup>1</sup>FOM-AMOLF, Amsterdam, Netherlands; <sup>2</sup>University of Heidelberg, Heidelberg, Germany
- WP 194 Enhancement of Au and Silica Nanoparticle Matrices for Tissue Imaging utilizing MALDI-TOF MS;

  Jeremy D. Post<sup>1</sup>; Alice Delvolve<sup>1</sup>; J. Albert Schultz<sup>2</sup>;

  Steven Oldenburg<sup>3</sup>; Amina S. Woods<sup>4</sup>; <sup>1</sup>NIH/NIDA-IRP, Baltimore, MD; <sup>2</sup>Ionwerks, Inc., Houston, TX;

  <sup>3</sup>nanoComposix, San Diego, CA; <sup>4</sup>NIDA IRP, NIH, Baltimore, MD
- WP 195 LC-SIMS: The Doors Wide Open for Biological Applications of SIMS in Imaging Mass

**Spectrometry;** <u>Luke MacAleese</u>; Leendert A. Klerk; Donald F. Smith; Marc C. Duursma; Ron M.A. Heeren; *FOM Institute AMOLF, Amsterdam, Netherlands* 

# **ION MOBILITY, 196 - 217**

- WP 196 Gating in Ion Mobility Spectrometry; Bill Siems<sup>1</sup>; Eric J. Davis<sup>1</sup>; Kristyn Roscioli<sup>1</sup>; Christina Crawford<sup>1</sup>; Herbert H Hill<sup>2</sup>; <sup>1</sup>Washington State University, Pullman, WA; <sup>2</sup>Washington State University, Pullman, WA
- WP 197 **Tissue Imaging of Pharmaceuticals by Ion Mobility**Mass Spectrometry; Stacey R. Oppenheimer<sup>1</sup>; <u>Tasneem Bahrainwala</u><sup>2</sup>; Emmanuelle Claude<sup>2</sup>; <sup>1</sup>Pfizer, Groton,
  CT; <sup>2</sup>Waters Corporation, Beverly, MA
- WP 198 Development and Evaluation of a DMS-Based
  Method for the Detection of Insecticides; Erick
  Molina<sup>1</sup>; Erkinjon Nazarov<sup>3</sup>; Ulrich R. Bernier<sup>2</sup>; Richard
  A. Yost<sup>1</sup>; <sup>1</sup>University of Florida, Gainesville, FL;
  <sup>2</sup>USDA-ARS-CMAVE, Gainesville, FL; <sup>3</sup>Sionex, Bedford,
  MA
- WP 199 Ion/Ion Reaction Effects on the Conformation of Proteins, Peptides, and Small Biomolecules; Derrick

  L. Morast<sup>1</sup>; R. Sam Houk<sup>1</sup>; Gregg Schieffer<sup>1</sup>; Ethan R. Badman<sup>2</sup>; Jowa State University, Ames, IA; Hoffmann-La Roche Inc., Nutley, NJ
- WP 200 Structural Transitions of the [M + 10H] <sup>10+</sup> of Ubiquitin by Overtone Mobility Spectrometry (OMS); Sunyoung Lee; Fabiane M Nachtigall; David E. Clemmer; Indiana University, Bloomington, IN
- WP 201 Hydrogen/Deuterium Exchange of Mobility Selected
  Ubiquitin Ions Using a High-Resolution Circular Ion
  Mobility Spectrometry Instrument in Ring-Down
  Mode; Rebecca S. Glaskin; Samuel Merenbloom; David
  E. Clemmer; Indiana University, Bloomington, IN
- WP 202 **Developing Techniques for Characterizing the Serum**Glycoproteome with LC-IMS-MS; Nicholas A
  Pierson; Huilin Shi; Stephen Valentine; David E.
  Clemmer; Indiana University, Bloomington, IN
- WP 203 Differential Mobility Spectrometer Coupled with LTQ FT to Evaluate Improvement of Proteomic Coverage of Complex Protein Mixtures; Sergei Ilchenko<sup>1</sup>; Daniela M Schlatzer<sup>1</sup>; Mark Chance<sup>1</sup>; Evgeny V Krylov<sup>2</sup>; Erkinjon Nazarov<sup>2</sup>; I Case Western Reserve University, Cleveland, OH; Sionex Corp., Bedford, MA
- WP 204 Accurate and Reproducible Reduced Mobility Values in Ion Mobility Spectrometry; Christina L. Crawford<sup>1</sup>; Roberto Fernandez Maestre<sup>1</sup>; Charles S. Harden<sup>2</sup>; Vincent M. McHugh<sup>3</sup>; William F. Siems<sup>1</sup>; Herbert H. Hill<sup>1</sup>; <sup>1</sup>Washington State University, Pullman, WA; <sup>2</sup>SAIC/ECBC Operations, Aberdeen Proving Ground, MD; <sup>3</sup>US Army Edgewood Chem Bio Center, Aberdeen Proving Ground, MD
- WP 205 **Developing IMS-IMS-IMS-MS for Analysis of Large Protein Complexes**; Natalya Atlasevich; Joshua Maze;
  Brian Bohrer; Martin Jarrold; David E. Clemmer;
  Indiana University, Bloomington, IN
- WP 206 Ion Mobility-Mass Spectrometry: A Novel Approach to the Analysis of Gold Monolayer Protected Clusters; Kellen M. Harkness; David E. Cliffel; John A. Mclean; Vanderbilt University, Nashville, TN
- WP 207 Accelerated Detection of Biomarkers Using DMS-Prefiltered Mass Spectrometry; Stephen L Coy<sup>1</sup>; Evgeny V Krylov<sup>1</sup>; Erkinjon Nazarov<sup>2</sup>; <sup>1</sup>Sionex Corp., Bedford, MA; <sup>2</sup>Sionex, Bedford, MA
- WP 208 Middle-Down Sequencing of Monoclonal Antibodies by Ion Mobility Q-TOF Mass Spectrometry;

  Dhanashri Bagal<sup>1</sup>; Himanshu Gadgil<sup>2</sup>; Paul Schnier<sup>1</sup>;

  Amgen, Thousand Oaks, CA; Amgen Inc, Seattle, WA

- WP 209 Ion Mobility-Mass Spectrometry Measurements of Insulin; Rune Salbo¹; Claus G Nielsen¹; Ingrid, V. Pettersson¹; Kim F. Haselmann¹; Iain D G Campuzano²; Peter, K. Nielsen¹; Helle Naver¹; ¹Novo Nordisk, Maaloev, Denmark; ²Waters Corporation, Manchester, UK
- WP 210 Collision Cross-Section Calculation of Serine
  Octamer Clusters Using Travelling Wave-Based
  Ionmobility Mass Spectrometer; Gustavo H M F
  Souza<sup>12</sup>; Marcos N Eberlin<sup>3</sup>; \*\*Waters Corporation, Sao
  Paulo, Brazil; \*\*2Waters Corporation, Manchester, UK;
  \*\*ThomSon Lab UNICAMP, Campinas, SP, Brazil\*\*
- WP 211 Determining the Structures and the Assembly of AAA+ Motor, Sliding Clamp Loader By Ion Mobility and Tandem Mass Spectrometry; Ahyoung Park; Brandon Ruotolo; Argyris Politis; Daniel Barsky; Carol Robinson; University of Cambridge, Cambirdge, UK
- WP 212 **Development of a Circular Drift Tube for High**Resolution Ion Mobility Spectrometry; Samuel I.

  Merenbloom; Rebecca S. Glaskin; Zachary B. Henson;
  David E. Clemmer; Indiana University, Bloomington, IN
- WP 213 Periodic Focusing Field Electrodes for High Resolution Ion Mobility Spectrometry; Ryan Blase; Kent Gillig; David H. Russell; Texas A&M University, College Station, TX
- WP 214 A Different Way of Measuring Ion Mobility for Absolute Cross Sections at Ultra-High Resolution TOF MS; Gökhan Baykut; Oliver von Halem; Oliver Raether; Bruker Daltonik GmbH, Bremen, Germany
- WP 215 Identifying Human Plasma N-linked Glycan Isomers
  Using Combined Ion Mobility-Mass Spectrometry
  and Molecular Modeling Methods; Manolo D.
  Plasencia; V. Blake Champlin; David E. Clemmer;
  Indiana University, Bloomington, IN
- WP 216 Separation of Isomeric Carotenoids Using
  Atmospheric Pressure Chemical Ionization Ion
  Mobility Spectrometry-Time-of-Flight Mass
  Spectrometry; Linlin Dong<sup>1</sup>; Roderick Davis<sup>2</sup>; Richard
  B. Van Breemen<sup>1</sup>; <sup>1</sup>University of Illinois College of
  Pharmacy, Chicago, IL; <sup>2</sup>Univ.of Illinois at Chicago
  Research Resources Ctr, Chicago, IL
- WP 217 Application of Ion Mobility Techniques in the Analysis of the Impurities in a Mixture of Liquid Crystals; Sung-Chan Jo<sup>1</sup>; Kyoung-Wook Kim<sup>2</sup>; Weonsik Oh<sup>1</sup>; Samsung Electronics Co., Ltd., Yongin, South Korea; Waters Korea Limited, Seoul, Korea

# **QUANTITATION: SMALL MOLECULE, 218 - 246**

- WP 218 LC/MS/MS Determination of Emtricitabine and Tenofovir in Human Plasma; Lina Tang; Hsun-Wen Chou; Venketraman Junnotula; Yuwen Zhao; Kris Singleton; Jamie Zhao; Yuan-shek Chen; Kumar Ramu; QPS, LLC, Newark, DE
- WP 219 Evaluation of Free and Protein-Bound 3-Nitrotyrosine in Human Plasma By Isotope Dilution LC-QqQ with an Artifactual Nitration-Free Proteolysis; Thierry Delatour; Janique Richoz; Christophe Cavin; Aurélien Desmarchelier; Nestle Research Center, Lausanne, Switzerland
- WP 220 Studies of Intestinal Absorption and Serum Levels of Novel Chemopreventive Agents; Soyoun Ahn<sup>1</sup>; Mark S Cushman<sup>2,2</sup>; John M Pezzuto<sup>2</sup>; Richard B. Van Breemen<sup>1</sup>; <sup>1</sup>University of Illinois, Chicago, IL; <sup>2</sup>Purdue University, West Lafayette, IN
- WP 221 Increasing the Selectivity of Clenbuterol Detection in Urine Samples By Using MS3 on a Hybrid Quadrupole-Linear Ion Trap; Mauro Aiello; Rolf

WP 222

#### WEDNESDAY POSTERS

- Kern; Beth Fernandez; Loren Olson; Applied Biosystems, San Jose, CA Software Assisted Chiral Chromatographic Method Development for the Quantitation of Four Chiral
- Drugs in Human Plasma using LC/MS/MS; Patrick Bennett; Min Meng; Lisa Rohde; Tandem Labs, Salt Lake City, UT
- WP 223 Application of High pH Mobile Phase in LC-ESI(+)/MS/MS Under HILIC Mode to Reach Optimal Sensitivity for Bioanalysis; Eugénie-Raphaëlle Bérubé; Jean-Nicholas Mess; Milton Furtado; Fabio Garofolo; Algorithme Pharma Inc., Laval (Montreal), Quebec, Canada
- WP 224 A Novel Algorithm for Quantitative LC Peak Integration; Lyle Burton; Gordana Ivosev; Lau Adam; Ron Bonner; MDS Analytical Tech, Sciex, Concord, Canada
- WP 225 Trace Analysis (ppt) Via LC/MS/MS to Assess
  Removal of Various Pharmaceutical Compounds by
  Activated Carbon Based Drinking Water Filters;
  Hong Jian Dai; Todd Branch; Peter Beerse; Stanley
  Cummins; Tom Huggins; Procter & Gamble, Mason,
  OH
- WP 226 Comparison of Linear Ion Trap and Triple Quadruple Mass Analyzer for Quantitation: An Antibiotics Case Study; Susie Dai<sup>1,2</sup>; Timothy Herrman<sup>1,2</sup>; <sup>1</sup>Office of the Texas State Chemist, College Station, TX; <sup>2</sup>Texas A&M University, College Station, TX
- WP 227 Development and Validation of an LC-MS/MS
  Method for Farnesol Quantitation in Candida
  Albicans Biofilms; Marie-Claude Denis; Karine Venne;
  Annie Leduc; Jean Barbeau; Alexandra Furtos;
  Universite de Montreal, Montreal, Canada
- WP 228 HPLC/MS/MS with In-Source Collision-Induced Dissociation for Direct Measurement of PEGylated Compounds in Biological Matrices; Mark Dreyer<sup>1</sup>; Linda Chen<sup>1</sup>; Dale Schoener<sup>2</sup>; Oanh Dang<sup>2</sup>; <sup>1</sup>Elan Pharmaceuticals, South San Francisco, CA; <sup>2</sup>Alta Analytical Laboratory, El Dorado Hills, CA
- WP 229 Quantification of Illegal Drugs in Urine Using Magnetic Nanoprobes and MALDI-TOF MS; Chi-Yi Ho¹; Po-Chiao Lin²; Chun-Cheng Lin²; Ying-Wei Lu²; Mei-Chun Tseng³; Yu-Ju Chen³; Ming-Ren Fuh¹; ¹Department of Chemistry, Soochow University, Taipei, Taiwan; ²Department of Chemistry, Tsing Hua University, Hsinchu, Taiwan; ³Institute of Chemistry, Academia Sinica, Taipei, Taiwan
- WP 230 **500 Discovery Samples a Day: Maximizing**Throughput and Minimizing Matrix Effects in
  Discovery Analysis; Rob Horton; Gerard Dalglish;
  Edward Brewer; Tandem Labs, West Trenton, NJ
- WP 231 Preparation of Quantum Dots and Concentration Measurements via ICP-MS for The Application of Neurotransmitter Sensing; Jong Sung Kim; Jeong Ha Yoo; Kyungwon University, Seongnam, South Korea
- WP 232 Summation of Multiple Transitions Monitoring in LC/MS/MS to Enhance Signal to Noise and to Reduce Variability; François Viel; Isabelle M. Levesque; Sebastien Gagne; Sylvain Lachance; Philippe Belanger; Jean Couture; Ann Levesque; Robert Masse; Anapharm, Québec, Canada
- WP 233 Quantitation without Standards via Electrosprayed Clusters: Determining Solution Molar Fractions of Peptides and Small Molecules; Ryan D. Leib; Tawnya

- G. Flick; Evan R. Williams; *University of California, Berkeley, CA*
- WP 234 Overcome Non-Phospholipid Related Matrix Effect and Continuing Improvement for the Quantification of Naltrexone and 6β-Naltrexol in Human Plasma by LC/MS/MS; Min Meng; Lin Tan; Troy Volker; Ryan Alder; Patrick Bennett; Tandem Labs, Salt Lake City, UT
- WP 235 A Unique Approach for 'Top down Analysis' of Melamine in Herbal Matrix Using HCD and High Resolution Mass Spectrometry; Ge Xiao Wei<sup>1</sup>; Nargund Sandy<sup>2</sup>; Martina Monique<sup>2</sup>; Health Sciences Authority, Singapore, Singapore; Alpha Analytical [S] Pte Ltd, Singapore, Singapore
- WP 236 The Simultaneous Detection of Metabolites and Quantification of Drug Molecules in Bioanalytical Assays; Rob Plumb<sup>1</sup>; Paul Rainville<sup>1</sup>; Joanne Mather<sup>2</sup>; Ian Wilson<sup>3</sup>; <sup>1</sup>Waters, Milford, MA; <sup>2</sup>waters corporation, Milford, MA; <sup>3</sup>Astra Zeneca, Macderfield, UK
- WP 237 Ways to Handle Matrix Effect in Quantitative Bio-Analysis in Real Time Analysis; Ashutosh Pudage; Noel Gomes; Accutest Research Laboratory, Navi Mumbai, India
- WP 238 Hydrophobic Interaction Chromatography (HILIC)
  Analysis of 6MPR For Targeted Drug Delivery to the
  Brain Using Gold Nanoparticles (AuNP) via
  LC/MS/MS; Brian Rago; Julie Poe; Lisa Buchholz;
  Ayman El-Kattan; Charles Rotter; Manthena Varma;
  Paul Nkansah; Pfizer, Groton, CT
- WP 239 Monitoring Matrix Interferences in Biological Samples Utilizing Dual Scan MRM Mode Mass Spectrometry; Paul Rainville<sup>1</sup>; Robert Plumb<sup>2</sup>; Joanne Mather<sup>3</sup>; \*Waters, Milford, MA; \*Imperial College, London, UK; \*waters corporation, Milford, MA
- WP 240 Development of the New Method for Quantitation and Screening Analysis of Organic Acids by Means of Using IC/MS/MS; Kaori Saito<sup>1</sup>; Tomoko Hamasaka<sup>1</sup>; Yoko Yamagishi<sup>1</sup>; Shigeru Sakamoto<sup>1</sup>; Takahiro Suzuki<sup>2</sup>; \*\*Ithermo Fisher Scientific K.K., Yokohama, Japan; \*\*2Nippon Dionex K.K., Tokyo, Japan
- WP 241 Quantitative Bioanalysis using Time of Flight Mass Spectrometry and Fast Liquid Chromatography; Gunnar Stenhagen; AstraZeneca R&D, Mölndal, Sweden
- WP 242 Mass Spectrometry of Polydisperse Samples: A
  Simple Step-by-Step Approach to Insure
  Quantitation; William E. Wallace; Charles M.
  Guttman; Kathleen M Flynn; National Institute of
  Standards & Technology, Gaithersburg, MD
- WP 243 Successful Applications of Autosampler Needle Seat Back-Flush to Reduce Carryover Using Common HPLC Hardware When Standard Washing Procedures Are Ineffective; Marie-Pierre Taillon; Nikolay Youhnovski; Simon Robert; Louis-Philippe Morin; Milton Furtado; Fabio Garofolo; Algorithme Pharma Inc., Laval (Montreal), Quebec, Canada
- WP 244 Quadratic Behavior in Standard Curves in LC-MS/MS Bioanalytical Assays: Is a Wide Curve Range the Root Cause? Long Yuan; Yunlin Fu; Anne-Francoise Aubry; Duxi Zhang; Bristol-Myers Squibb, Princeton, NJ
- WP 245 **Development of an Automation Assisted Generic Approach for LC-MS/MS Method Validation**; <u>Jie</u>

  <u>Zhang</u>; Shimin Wei; H Tom Smith; Francis Tse; <u>DMPK</u>,

  <u>Novartis Pharmaceuticals Corporation</u>, <u>East Hanover</u>,

  NJ

WP 246 **Multidimensional Molecular Identification by Laser** Control Mass Spectrometry; Xin Zhu; East Lansing,

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- WP 247 Evaluation of 3-Iodothyronamine (T1AM) in Cell Preparation, Tissue Homogenates and Biological Fluids by HPLC-ESI-MS-MS; Alessandro Saba<sup>1</sup>; Grazia Chiellini<sup>2</sup>; Sabina Frascarelli<sup>2</sup>; Sandra Ghelardoni<sup>2</sup>; Maja Marchini<sup>2</sup>; Andrea Raffaelli<sup>3</sup>; Riccardo Zucchi<sup>2</sup>; <sup>1</sup>University of Pisa - Chemistry Dept., Pisa, Italy; <sup>2</sup>University of Pisa - Medical School, Pisa, Italy; <sup>3</sup>CNR ICCOM, Pisa, Italy
- WP 248 Application of Diels-Alder Derivatization and 96 Well Plate Solid Phase Extraction to Increase the Throughput of 25-Hydroxyvitamin D3 Analysis; Pavel A. Aronov<sup>1</sup>; Jun Yang<sup>2</sup>; Laura M. Hall<sup>2</sup>; Charles B. Stephensen<sup>2</sup>; Bruce D. Hammock<sup>2</sup>; <sup>1</sup>Stanford, Stanford, CA; <sup>2</sup>University of California, Davis, Davis,
- WP 249 Rapid Analysis of Catecholamines and Metanephrines in Biological Fluids by Automated Online Solid-Phase Extraction LC/MS/MS; Sylvie Beaudet<sup>1</sup>; Martin Sibum<sup>2</sup>; Luce Boulanger<sup>3</sup>; <sup>1</sup>MDS Analytical Technologies, Concord, Canada; <sup>2</sup>Spark Holland Inc.,, Emmen, Netherlands; <sup>3</sup>CHUM St-Luc Hospital, Montreal, Canada
- WP 250 Development of a Reference Method for B6 Vitamer Pyridoxal 5'-Phosphate in Serum Using Isotope-**Dilution Liquid Chromatography-Electrospray Ionization Tandem Mass Spectrometry**; <u>Johanna E.</u> Camara; Karen W. Phinney; NIST, Gaithersburg, MD
- WP 251 Determination of Plasma Free Metanephrines by On-Line Extraction and Hydrophilic Liquid **Chromatography Coupled to Tandem Mass** Spectrometry; Karina Helena Morais Cardozo; Marlene Freitas Madeira; Fleury Medicine and Health, São Paulo, Brazil
- WP 252 Quantitation of Underivatized Acylcarnitines and **Acyl CoA Fatty Acid Esters in Rat Tissue Samples** Using Triple Quadrupole Mass Spectrometry; James Carlson<sup>1</sup>; Jenny Moshin<sup>1</sup>; Susan Leonard<sup>1</sup>; Yan Wang<sup>2</sup> Irving Wainer<sup>2</sup>; <sup>1</sup>Applied Biosystems, Framingham, MA; <sup>2</sup>NIH/NIA, Baltimore, MD
- WP 253 **High-Throughput Isotope-Dilution Liquid Chromatography-Tandem Mass Spectrometry Assay** for Simultaneous Measurement of Vitamins D2 and D3 25-Hydroxy Metabolites in Human Serum; Valdemir Melechco Carvalho; Odete Hirata Nakamura; Marlene de Freitas Madeira; José Gilberto Vieira; Fleury Medicine and Health, Sao Paulo, Brasil
- WP 254 **Detection of Specific Porphyrias Using Tandem Mass** Spectrometry; Autumn W. Burns; John Choiniere; Frantisek Turecek; Michael H. Gelb; C. Ronald Scott; University of Washington, Seattle, WA
- WP 255 Simple and Fast Method for Determination of Acetaminophen in Serum; Jose Luiz Costa<sup>1</sup>; Rafael Lanaro<sup>2</sup>; Anna Slyvia Ferrari Marques<sup>1</sup>; Helio Martins<sup>1</sup>; <sup>1</sup>Applied Biosystems, Sao Paulo, Brazil; <sup>2</sup>Poison Control Center, Faculty of Medical, Campinas, Brazil
- WP 256 A LC-MS/MS Platform for the Simultaneous TDM **Analysis of Opiates and Benzodiazepines with Direct Urine Injection**; <u>Christopher L. Esposito</u><sup>1</sup>; Francois A. Espourteille<sup>2</sup>; Matthew Berube<sup>2</sup>; <sup>1</sup>*Thermo Scientific*, Franklin, MA; <sup>2</sup>Thermo Fisher Scientific, Franklin, MA
- WP 257 Free and Total Sialic Acid in CSF by UPLC-MS/MS; Sabrina Forni; Xiaowei Fu; Raphael Schiffmann;

- Lawrence Sweetman; Inst. of Metabolic Disease, Baylor Res. Institute, Dallas, Texas
- WP 258 Analysis of Antidepressants and Neuroleptics in Serum/Plasma by LC/MS/MS; Tanya Gamble<sup>2</sup>; Tania A. Sasaki<sup>1</sup>; Lisa Sapp<sup>1</sup>; <sup>1</sup>Applied Biosystems, Foster City, CA; <sup>2</sup>Applied Biosystems/MDS Analytical Technologies, Concord, Canada
- WP 259 Quantification of Plasma S-Adenosyl Homocysteine and S-Adenosyl Methione by Stable Isotope Dilution Positive Ion ESI LC/MS/MS with On-Line Concentration; <u>David Hasman</u><sup>1,2</sup>; Sheila M Innis<sup>2</sup>; <sup>1</sup>Procyon Research Inc., Vancouver, Canada; <sup>2</sup>University of British Columbia, Vancouver, BC Canada
- WP 260 Analysis of Leukotriene B4 and Cysteinyl-Leukotrienes in Human Sputum; Gloria P. Lazar; Xiaoyao Xiao; Arnaldo Pica-Mendez; Omar Laterza; Wesley K. Tanaka; Merck & Company, Inc., Rahway,
- WP 261 Automated SPE-LC/MS/MS Assay for 25-OH Vitamin D Metabolites in Blood; Kimberly Eaton<sup>1</sup>, M. P. George<sup>2</sup>; Tony Brand<sup>2</sup>; Kimberly Gamble<sup>3</sup>; <u>Ken</u> Lewis<sup>1</sup>; <sup>1</sup>OpAns, LLC, Durham, NC; <sup>2</sup>Agilent Technologies, Santa Clara, CA; <sup>3</sup>MicroLiter Analytical Supplies, Inc., Suwanee, GA
- WP 262 A New Software Application Enabling User Walk-up LC-MS Quantification of Immunosuppressants for the Clinical Laboratory; Dennis G. Nagtalon; Thermo Fisher Scientific, San Jose, CA
- WP 263 **Endogenous Prednisolone and Prednisone** Interference Elucidation by Linear Ion Trap in a Clinical Assay; Brian C Netzel; Ravinder J. Singh; Molly A. VanNorman; Tania A. Sasaki<sup>2</sup>; *Mayo Clinic*, Rochester, MN; <sup>2</sup>Applied Biosystems
- WP 264 **Improved Sensitivity in Mass Spectrometric Ouantification of Cardiolipin in Human Serum by** HPLC/ESI-MS; Elizabeth W. Ogbonna<sup>1</sup>; Hee-Yong Kim<sup>2</sup>; Alfred L. Yergey<sup>1</sup>; Peter S. Backlund<sup>1</sup>; <sup>1</sup>NICHD/NIH, Bethesda, MD; <sup>2</sup>NIAAA/NIH, Bethesda,
- WP 265 An Isotope-Dilution GC/MS Method for the Quantitation of 25-Hydroxy-Vitamin D<sub>3</sub> in Human Serum; Anna M. Przyborowska<sup>1</sup>; Graham D. Carter<sup>2</sup>; Julia C. Jones<sup>2</sup>; John M. Halket<sup>1,2</sup>; <sup>1</sup>King's College London, London, UK; <sup>2</sup>Imperial College Healthcare NHS Trust, London, UK
- WP 266 In-Source Water Loss As a Source of Analytical Error in Vitamin D LC/MS/MS Quantitative Analysis; Eduard Rogatsky; Daniel Stein; Albert Einstein College of Medicine, Bronx, NY
- WP 267 Simultaneous Determination of Alpha-Aminoadipic Semialdehyde, Piperideine-6-Carboxylate, and Pipecolic Acid in Human Plasma by Liquid Chromatography-Mass Spectrometry; Katerina Sadilkova<sup>1</sup>; Si Houn Hahn<sup>1,2</sup>; <sup>1</sup>Seattle Children's, Seattle, WA; <sup>2</sup>University of Washington, Seattle, WA
- WP 268 Method Development for the Determination of 25-Hydroxyvitamin D3 and 25-Hydroxyvitamin D2 in **Serum Using Isotope Dilution Liquid** Chromatography-Tandem Mass Spectrometry; Susan Tai; NIST, Gaithersburg, MD
- WP 269 Plasma Free Metanephrine and Normetanephrine **Quantitation Using On-line Sample Extraction** Coupled with Tandem Mass Spectrometry; Yang Shi; Catherine Lafontaine; Tim Haney; Joseph J. Takarewski; François A. Espourteille; Thermo Fisher Scientific, Franklin, MA

- WP 270 Increased Throughput of Vitamin D Analysis Using a Multiple Parallel LC-MS System; Adrian Taylor;
  David Cox; Min J. Yang; John Gibbons; MDS Analytical Technologies, Concord, Canada
- WP 271 Fast Analysis of 15 Endogenous Estrogens using Positive Ion Electrospray with Cumulative Multicolumn Sequential Chromatography for Low Femtogram Analysis; Timothy D. Veenstra<sup>1</sup>; Xia Xu<sup>1</sup>; Haleem Isaaq<sup>1</sup>; King Chan<sup>1</sup>; Robert Classon<sup>2</sup>; William A Hedgepeth<sup>2</sup>; <sup>1</sup>SAIC-Frederick, Inc., Frederick, MD; <sup>2</sup>Shimadzu Scientific Instruments, Inc, Columbia, MD
- WP 272 A Novel Derivatisation Reagent to Enhance the Detection Characteristics of Keto-Steroids via LC-MS; Brian L Williamson; Marjorie Minkoff; Scott B. Daniels; Subhakar Dey; Babu Purkayastha; Applied Biosystems, Framingham, MA
- WP 273 High-Throughput Analysis of Serum 5&alpha-Dihydrotestosterone by 2D-LC-MS/MS; Bingfang Yue<sup>1</sup>; Mark M. Kushnir<sup>1</sup>; A Wayne Meikle<sup>1,2</sup>; Alan L. Rockwood<sup>1,3</sup>; <sup>1</sup>ARUP Laboratories, Salt Lake City, UT; <sup>2</sup>Dept. Medicine and Pathology, University of Utah, Sal Lake City, UT; <sup>3</sup>Dept. of Pathology, University of Utah, Salt Lake City, UT
- WP 274 Simultaneous Screening, Quantitation and Confirmation of Regulated Chemicals for the Treatment of Erectile Dysfunction in Dietary Supplements; Hwami Lee<sup>1</sup>; Hansoon Kwon<sup>3</sup>; Sunghoon Yeo<sup>3</sup>; Jiehui Hu<sup>2</sup>; <u>Huaien Zhu</u><sup>2</sup>; Yongming Xie<sup>2</sup>; Sanghwa Kim<sup>3</sup>; Myunghee Kang<sup>1</sup>; Youngmi Jang<sup>1</sup>; 

  <sup>1</sup>Korea Food & Drug Administration, Incheon, South Korea; <sup>2</sup>Applied Biosystems 1, Shanghai, China; 
  <sup>3</sup>Applied Biosystems, Seoul, South Korea
- WP 275 Detection and Quantification of the Endocrine Disruptor Clomiphene Citrate in Serum and Meconium by LC-ESI-MSn; Justin Lygrisse; Kelsey Witherspoon; Michael J. Van Stipdonk; Wichita State University, Wichita, KS

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- WP 276 Methodological Development for Mural Painting
  Ageing Study; Sophie Dallongeville; Sylvia Turrell;
  Christian Rolando; Caroline Tokarski; Univ. des
  Science/Tech de Lille, Villeneuve D'ascq, France
- WP 277 Proteomics and Redox Proteomics Analyses to
  Understand the Role of Oxidative Stress in
  Immunosenescence of Aging Mice; Renã A. Sowell; D.
  Allan Butterfield; University of Kentucky, Lexington, KY
- WP 278 **Top-Down Identification of Protein Modifications**Induced by Cigarette Smoke Condensate; Pauline Le
  Faouder<sup>1</sup>; Iman Emami<sup>2</sup>; Caroline Tokarski<sup>1</sup>; Christian
  Rolando<sup>1</sup>; <sup>1</sup>Univ. des Science/Tech de Lille, Villeneuve
  D'ascq, France; <sup>2</sup>Biosyntech, Paris, France
- WP 279 Post-Translational Modifications of Model Proteins with 4-Hydroxynonenal, a Quantitative Analysis of Reactivity at Specific Sites; Qingyuan Liu; Scott Gronert; Virginia Commonwealth University, Richmond,
- WP 280 Identification and Characterization of 3-Nitrotyrosine Modified Proteins in Cerebrospinal Fluid; <u>Ashley Beasley</u><sup>1</sup>; Avindra Nath<sup>1</sup>; Robert J. Cotter<sup>2</sup>; <sup>1</sup>Johns Hopkins University School of Medicine, Baltimore, MD; <sup>2</sup>Middle Atlantic MS Laboratory, Baltimore, MD
- WP 281 Modification Specific Proteomics: Specific Enrichment and Identification of Carbonylated Sites in Proteins; Angela Pereira Da Rocha; Adelina

- Rogowska-Wrzesinska; Kenneth Bendix Jensen; Peter Roepstorff; *University of Southern Denmark, Odense, Denmark*
- WP 282 Primary Sequence and Site-Selective Hydroxylation of Prolines in Isoforms of the Peanut Allergen
  Protein Ara h 2; Jinxi Li¹; Kevin J. Shefcheck²; John H. Callahan²; Catherine Fenselau¹; ¹University of Maryland, College Park, MD; ²FDA/CFSAN, College Park, MD
- WP 283 High-Content Quantitation of the S-Nitrosylated Proteins in Parkinson's Disease Paradigms; Fanjun Meng<sup>1,2</sup>; Fan Wei<sup>2</sup>; Siqi Liu<sup>2</sup>; Zezong Gu<sup>1,3</sup>; <sup>1</sup>University of Missouri-Columbia School of Medicine, Columbia, MO; <sup>2</sup>Chinese Academy of Sci Beijing Genomics Institute, Beijing, China; <sup>3</sup>Burnham Institute for Medical Research, La Jolla, CA
- WP 284 Optimization of a 2DE-Based Biotin Switch Method for Proteomics Analysis of Nitrosylated Proteins;

  Changgoog Wu; Tong Liu; Cexiong Fu; Wei Chen;
  Mohit Jain; Hong Li; UMDNJ, Newark, NJ
- WP 285 Identification of Sites and Tissue-Dependent Protein
  Targets for Posttranslational Modifications by 4Hydroxy-2-Nonenal, an End-Product of Lipid
  Peroxidation, in the Mitochondria; Navin Rauniyar;
  Katalin Prokai-Tatrai; Laszlo Prokai; UNT Health
  Science Center, Fort Worth, TX
- WP 286 Characterization and Performance of a
  Multicomponent Protein Mixture for the Analysis of
  Tyrosine Nitration Using Several Mass Spectrometry
  Platforms; Bensheng Li; Birgit Schilling; Jason M.
  Held; Bradford W. Gibson; Buck Institute for Age
  Research, Novato, CA 94945
- WP 287 Quantitative Profiling of Site-Specific Hydroxylation on the Hypoxia-Inducible Factors HIF1&alpha and HIF2α Dean E. Mcnulty; Melissa B. Pappalardi; Lusong Luo; Roland S. Annan; GlaxoSmithKline, King of Prussia, PA
- WP 288 Nitrated Fibrinogen: A Novel Risk Factor for Deep Venous Thrombosis; Marissa Martinez<sup>1</sup>; Giannis Parastatidis<sup>2</sup>; Ian A. Blair<sup>3</sup>; Harry Ischiropoulos<sup>2</sup>; 

  <sup>1</sup>University of Pennsylvania, Philadelphia, PA; 

  <sup>2</sup>Childrens Hospital of Philadelphia, Philadelphia, PA; 

  <sup>3</sup>Univ. of Penn/SOM/Pharmacol, Philadelphia, PA
- WP 289 Label-Free Strategy for Site-Specific Quantitation of S-Nitrosylome; Hsiao-Chiao Chou<sup>1,3</sup>; Yi-Ju Chen<sup>2,3</sup>; Wei-Chi Ku<sup>3</sup>; Yu-Ju Chen<sup>3</sup>; <sup>1</sup>Department of Chemistry, NTU, Taipei City, Taiwan; <sup>2</sup>IBS, National Taiwan University, Taipei City, Taiwan; <sup>3</sup>Institute of Chemistry, Academia Sinica, Taipei City, Taiwan
- WP 290 A Strategy for Direct Identification of Protein S-Nitrosylation Sites by Quadrupole Time-of-Flight Mass Spectrometry; Tong Liu; Yan Wang; Changgong Wu; Hong Li; UMDNJ, Newark, NJ
- WP 291 Peroxynitrite-Mediated Oxidative Post-Translational Modifications of Mitochondrial Complex II in the Post-Ischemic Myocardium; Liwen Zhang; Chwen-Lih Chen; kari. B Green-Church; Yoeng-Renn Chen; Ohio State University, Columbus, OH
- WP 292 Mass Spectrometry-Based Site-Specific Identification of S-Nitrosylome in Cardiovascular System; Yi-Ju Chen<sup>1,2</sup>; Hsiao-chiao Chou<sup>2,3</sup>; Wei-Chi Ku<sup>2</sup>; Kay-hooi Khoo<sup>1,4</sup>; Yu-Ju Chen<sup>2</sup>; <sup>1</sup>IBS, National Taiwan University, Taipei City, Taiwan; <sup>2</sup>Institute of Chemistry, Academia Sinica, Taipei City, Taiwan; <sup>3</sup>Institute of Chemistry, National Taiwan University, Taipei City, Taiwan; <sup>4</sup>IBC, Academia Sinica, Taipei City, Taiwan

- WP 293 Detection of Oxidation-Associated in vivo
  Carbonylation of Biologically Significant Proteins
  during Early Development of Zebrafish Embryos;
  Tatjana Talamantes; Navin Rauniyar; Katalin ProkaiTatrai; Laszlo Prokai; University of North Texas Health
  Science Center, Fort Worth, Texas
- WP 294 Analysis of Arginine and Lysine Methylation using Electron Transfer Dissociation Mass Spectrometry and Peptide Separations at Neutral pH; Ambrosius PL Snijders; Ming-Lung Hung; Stuart A Wilson; Mark J Dickman; University of Sheffield, Sheffield, UK
- WP 295 Towards the Development of a Method for the Quantitation of Methylation to Lysine Residues in Proteins; Anthony Berardinelli<sup>1</sup>; Bruce Snyder<sup>2</sup>; Amanda Bryant-Friedrich<sup>1</sup>; Wendell P. Griffith<sup>1</sup>; 

  <sup>1</sup>University of Toledo, Toledo, OH; <sup>2</sup>Emmanuel Christian High School, Toledo, OH
- WP 296 **Post-Translational Modifications on the Subunit p65 of NFkB**; Benlian Wang<sup>1</sup>; Tao Lu<sup>2</sup>; Masaru Miyagi<sup>1</sup>;
  George R. Stark<sup>2</sup>; Mark Chance<sup>1</sup>; <sup>1</sup>Case Western Reserve University, Cleveland, OH; <sup>2</sup>Lerner Research Institute, Cleveland, OH
- WP 297 An Unusual Case Study: MS/MS Spectrum of a Lysine-Methylated Peptide Looks Almost Perfectly Like That of a Serine Methylated Peptide; Junmei Zhang¹; Yue Chen²; Zhihong Zhang²; Joanna Wysocka³; Yingming Zhao⁴; ¹University of Texas Southwestern Medical Center, Dallas, TX; ²University of Chicago, Chicago, IL; ³Stanford University, Stanford, CA; ⁴The University of Chicago, Chicago, IL
- WP 298 Microtubules of Toxoplasma Gondii Contain C-Terminal Methylated α- and β-Tubulins; Hui Xiao¹; Kamal EI Bissati¹; pascal Verdier-Pinard²; Kami Kim¹; Berta Burd¹; Ruth Hogue Angeletti¹; Louis M. Weiss¹; ¹Albert Einstein College of Medcine, Bronx, NY; ²Aix-Marseille Université,, Marseille cedex, France
- WP 299 Screening of Ubiquitin K11 Linkage Specific Substrates by Quantitative Differential Display Proteomics Approach; Ping Xu<sup>1</sup>; Duc Duong<sup>1</sup>; Nicholas Seyfried<sup>2</sup>; D. Jessica Cheng<sup>1</sup>; John Rush<sup>3</sup>; Mark Hochstrasser<sup>4</sup>; Daniel Finley<sup>5</sup>; Junmin Peng<sup>1</sup>; <sup>1</sup>emory university, Atlanta, GA; <sup>2</sup>Department of Human Genetics, Atlanta, GA; <sup>3</sup>Cell Signaling Technology, Danvers, MA; <sup>4</sup>Yale University, New Haven, CT; <sup>5</sup>Harvard University, Boston, MA
- WP 300 Identification of EGF-Stimulation Specific PCM1
  Interaction Partners by Quantitative Proteomics;
  Vyacheslav Akimov; Kristoffer T. G. Rigbolt; Blagoy
  Blagoev; Uni. of Southern Denmark, Odense, Denmark
- WP 301 Characterisation of SUMOylated RanGAP1 by Ion Mobility/Time of Flight Mass Spectrometry; Mark Skehel; Helen Flynn; Sarah Maslen; Cancer Research UK, Hertfordshire, UK
- WP 302 Mapping Endogenous SUMO Sites: A Novel
  Approach Using ESI-MS and Modified Database
  Search with Common Search Engines; He-Hsuan
  Hsiao¹; Erik Meulmeester²; Benedikt T.C. Frank³;
  Frauke Melchior²; Henning Urlaub¹; IBioanalytical
  Mass Spectrometry Group, MPIbpc, Goettingen,
  Germany; Faculty of Medicine, University of
  Goettingen, Goettingen, Germany; Department of NMR
  Based Structural Biology, MPIbpc, Goettingen,
  Germany
- WP 303 Proteomic Analysis of SUMOylated Proteins in Mammalian Cells; Xiaoyan Liu; Fujian Zhang; Jianjun

- Zhai; Haining Zhu; University of Kentucky, Lexington, KY
- WP 304 A Quantitative Proteomics Approach to Characterize A Cellular TDP-43 Proteinopathy Model; Nicholas Seyfried<sup>1,3</sup>; Yair M. Gozal<sup>2,3</sup>; Qiangwei Xia<sup>1,3</sup>; Duc Duong<sup>1,3</sup>; Allan I. Levey<sup>2,3</sup>; James J. Lah<sup>2,3</sup>; Junmin Peng<sup>1,3</sup>; Department of Human Genetics, Atlanta, GA; Department of Neurology, Atlanta, GA; Emory University, School of Medicine, Atlanta, GA
- WP 305 Quantitative Identification of Acyl Modifications in SDS Resistant Pellets of S. Cerevisiae; Hongying Zhong; Jianjian Li; Yingxia Yue; Central China Normal University, Wuhan, China
- WP 306 Probing Huntingtin Palmitoylation Sites by Mass Spectrometry; Fiona BJ Young<sup>2,3</sup>; Michael R Hayden<sup>2,3</sup>; Bernd O Keller<sup>1,3</sup>; <sup>1</sup>University of British Columb, Vancouver, Canada; <sup>2</sup>UBC-CMMT, Vancouver, BC; <sup>3</sup>UBC-Child&Family Res. Institute, Vancouver, BC
- WP 307 **GPIomics: Global Analysis of**Glycosylphosphatidylinositol (GPI)-Anchored
  Molecules of Trypanosoma cruzi by Tandem Mass
  Spectrometry; Ernesto S. Nakayasu<sup>1</sup>; Dmitry V.
  Yashunsky<sup>2</sup>; Lilian L. Nohara<sup>1</sup>; Ana C.T. Torrecilhas<sup>3</sup>;
  Andrei V. Nikolaev<sup>2</sup>; <u>Igor C. Almeida</u><sup>1</sup>; <sup>1</sup>University of
  Texas at El Paso, El Paso, TX; <sup>2</sup>University of Dundee,
  Dundee, UK; <sup>3</sup>University of Sao Paulo, Sao Paulo,
  Brazil
- WP 308 Identification and Profiling of Novel Fatty Acid
  Modifications to Lens Major Intrinsic Protein AQP0;
  Zhen Wang¹; Danielle B Gutierrez²; Angus C Grey¹;
  Kevin L Schey¹; Vanderbilt University, Nashville, TN;

  2Medical University of South Carolina, Charleston, SC

# **INSTRUMENTATION: NEW CONCEPTS, 309 - 328**

- WP 309 Characterization of the "Ion-CCD" Used as Position Sensitive Detector for Charged Particles; Omar Hadjar; Gottfried Kibelka; Scott Shill; Scott Kassan; Chad Cameron; O.I. Analytical, Pelham, AL
- WP 310 Single Large Biomolecular Ion Detection; Chien-Hsun Chen<sup>1</sup>; Jung-Lee Lin<sup>1</sup>; Ming-Lee Chu<sup>2</sup>; Yi-Sheng Wang<sup>1</sup>; Chung-Hsuan Chen<sup>1</sup>; \*IGenomics Research Center, Academia Sinica, Taipei, Taiwan; \*Institute of Physics, Academia Sinica, Taipei, Taiwan
- WP 311 M2 Ion Detector for High Speed and Wide Dynamic Range; Motohiro Suyama; Hamamatsu Photonics K.K., Iwata, Japan
- WP 312 Improvements in Charge Detection Mass Spectrometry; Joshua Maze; Lloyd Zilch; John Smith; Nathan C. Contino; Haitao Tu; George E. Ewing; Martin Jarrold; Indiana University, Bloomington, IN
- WP 313 Increased Quantitative Throughput and Selectivity for Triple Quadrupole Mass Spectrometer Based Assays Using Intelligent SRM (iSRM); Reiko Kiyonami<sup>1</sup>; Alan E. Schoen<sup>1</sup>; Amol Prakash<sup>1</sup>; Huy Nguyen<sup>1</sup>; Scott Peterman<sup>1</sup>; Vlad Zabrouskov<sup>1</sup>; Charles T. Yang<sup>1</sup>; Dipankar Ghosh<sup>1</sup>; Kristi D. Akervik<sup>1</sup>; Nathalie Selevsek<sup>2</sup>; Andreas F Huhmer<sup>1</sup>; Bruno Domon<sup>2</sup>; 

  1 ThermoFisher Scientific, San Jose, CA; 2ETH Zurich, Zurich, Switzerland
- WP 314 Web-Enabled Management of an Ionization Source and Data Processing with the Apple iPod Touch;

  Peter Leopold<sup>1</sup>, Elizabeth Crawford<sup>2</sup>, Joseph Tice<sup>2</sup>;

  Michael Festa<sup>2</sup>, <sup>1</sup>BioAnalyte Inc., Portland, ME;

  <sup>2</sup>IonSense, Inc., Saugus, MA
- WP 315 RePlay® Combined with an Exclusion List Script Significantly Improves Number of Protein Assignments from Complex Proteomic Samples;

- <u>Daniel Eikel</u><sup>1</sup>; Christian Albers<sup>2</sup>; Geoffrey S. Rule<sup>3</sup>; Simon J. Prosser<sup>4</sup>; <sup>1</sup>AdvionBioSystems, Ithaca, NY; <sup>2</sup>Bruker Daltonik, Bremen, GERMANY; <sup>3</sup>Advion BioSystems, Salt Lake City, UT; <sup>4</sup>Advion BioSciences, Inc., Ithaca, NY
- WP 316 The Sensitivity of Laser-Induced Acoustic Desorption/Electron Ionization in a Fourier Transform Ion Cyclotron Resonance Mass Spectrometer; Zhicheng Jin<sup>1</sup>; Hilkka Kenttamaa<sup>2</sup>; 

  <sup>1</sup>Purdue University, West Lafayette, IN; <sup>2</sup>Chemistry Department, West Lafayette, IN
- WP 317 Development of Multiplexed Protein Separation and Identification Using Digital Microfluidics and Mass Spectrometry; Adam A. Stokes; Yifan Li; William Parkes; David J. Clarke; Pat Langridge-Smith; C. Logan Mackay; Anthony J. Walton; The University of Edinburgh, Edinburgh, Scotland
- WP 318 **Development of an Integrated High-Pressure**Microfluidic Nano-LC Platform; James Murphy;
  Geoff Gerhardt; Angela Doneanu; Jay Johnson; Joseph Michienzi; Keith Fadgen; Waters Corporation, Milford, MA
- WP 319 High Efficiency Mass Spectrometry Systems with Discontinuous Atmospheric Pressure Interface;
  Nicholas A. Charipar; Jason D. Harper; Matthew A. Kirleis; Wei Xu; Zheng Ouyang; Purdue University, Lafayette, IN
- WP 320 In-Source Atmospheric Pressure-Electron Capture Dissociation (AP-ECD): A New Tool for Structural Characterization of Peptides; Damon Robb<sup>1</sup>; Jason Rogalski<sup>1</sup>; Juergen Kast<sup>1</sup>; Michael Blades<sup>2</sup>; <sup>1</sup>University of British Columbia, Vancouver, Canada; <sup>2</sup>University of British Columb, Vancouver, BC
- WP 321 Online Bioaffinity- Electrospray Mass Spectrometry:
  Combining Molecular Identification and Bioaffinity
  Quantification in Biopolymer Interactions; Michael
  Przybylski<sup>1</sup>; Mihaela Dragusanu<sup>1</sup>; Stefan Slamnoiu<sup>1</sup>;
  Alina Petre<sup>1</sup>; Tingting Tu<sup>2</sup>; Michael L. Gross<sup>2</sup>;

  \*\*IUniversity of Konstanz, Konstanz, Germany;
  \*\*Washington University, Saint Louis, MO
- WP 322 Electrochemistry / Electrospray Mass Spectrometry for Investigation of Reaction Kinetics; Boguslaw Pozniak; Richard B. Cole; University of New Orleans, New Orleans, LA
- WP 323 Theoretical Studies of the Effect of Swirling Flow on Ion Focusing in a Coaxial Flow Electrospray Ion Source; Serguei Savtchenko<sup>2</sup>; Lisa Cousins<sup>2</sup>; Nasser Asgriz<sup>1</sup>; <sup>1</sup>University of Toronto, Toronto, ON, Canada; <sup>2</sup>IONICS Mass Spectrometry Group Inc., Toronto, ON
- WP 324 Simulations for Determining Mass Spectral Quality from μ-Cylindrical Ion Traps Using a Hard-Sphere Collision Buffer Gas Model; Friso H. W. van Amerom; Ashish Chaudhary; Tim Short; SRI International, St Petersburg, FL
- WP 325 A Carbon Nanotube Ionization Source for a Low Power Ion Trap Mass Spectrometer for Martian Organic Analysis; Theresa Evans-Nguyen<sup>1</sup>; Charles Parker<sup>2</sup>; Christina Hammock<sup>3</sup>; Vladimir M. Doroshenko<sup>4</sup>; Jeffrey Glass<sup>2</sup>; Luann Becker<sup>5</sup>; Robert J. Cotter<sup>1</sup>; <sup>1</sup>Johns Hopkins School of Medicine, Baltimore, MD; <sup>2</sup>Duke University, Durham, NC; <sup>3</sup>Johns Hopkins Applied Physics Lab, Laurel, MD; <sup>4</sup>MassTech, Inc., Columbia, MD; <sup>5</sup>Johns Hopkins University;, Baltimore, MD
- WP 326 A Rotating Ball LC/SALDI Interface Surface Activation and Analytical Performance; Sergey

- Alimpiev<sup>3</sup>; Alexander Gretchnikov<sup>2</sup>; Jan Sunner<sup>1</sup>; Sergey Nikiforov<sup>3</sup>; Yaroslav Simanovsky<sup>3</sup>; <sup>1</sup>University of Portsmouth, Portsmouth, UK; <sup>2</sup>Vernadsky Inst Geochem Anal Chem, Russ Acad Sci, Moscow, Russia; <sup>3</sup>Prokhorov General Physics Inst Russ Acad Sci, Moscow, Russia
- WP 327 Automated Vacuum Compatible Sample Positioning Device for Imaging Mass Spectrometry; Konstantin Aizikov<sup>1</sup>; Donald Smith<sup>2</sup>; David A. Chargin<sup>3</sup>; Sergei Ivanov<sup>3</sup>; David H. Perlman<sup>4</sup>; Tzu-yung Lin<sup>5</sup>; Nadezda P. Sargaeva<sup>5</sup>; Ron M.A. Heeren<sup>6</sup>; Peter B. O'Connor<sup>7</sup>; 

  <sup>1</sup>BUSM Mass Spectrometry Re, Boston, MA; <sup>2</sup>FOM-AMOLF, Amsterdam, Netherlands; <sup>3</sup>Fraunhofer CMI, Boston, MA; <sup>4</sup>Boston U. Sch. of Medicine, Boston, MA; <sup>5</sup>Boston University, Boston, MA; <sup>6</sup>FOM Inst. Atomic/Molecular Phy, Amsterdam, Netherlands; <sup>7</sup>University of Warwick, Coventry, UK
- WP 328 No Portable Mass Spec Required: Adaptive Sampling in the Field Using a Portable Automated Purification Robot with Lab MS ID; David Fries; Brian Gregson; Geran Barton; Stan Ivanov; U South Florida, St Petersburg, FL

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- WP 329 Compatability of UHPLC with MS, Are We More Productive? Marc Elliott<sup>1</sup>; Sean Mchugh<sup>1</sup>; Mark Woodruff<sup>2</sup>; Ken Butchart<sup>2</sup>; <sup>1</sup>Resolution Analytical Systems, Holland, MI; <sup>2</sup>Fortis Technologies Ltd, Neston,
- WP 330 Open Access with Open Arms: Implementation of a Single System that Meets the Varying Needs of Different Compounds; Zachary S Giles; GlaxoSmithKline, Rtp, NC
- WP 331 A Postcolumn Device for Signal Intensity
  Improvement of Peptides in TFA-containing Mobile
  Phase LC/MS; Nan-Hsuan Wang; Wan-Li Lee; GuorRong Her; National Taiwan University, Taipei, Taiwan
- WP 332 LC-MS/MS Bioanalysis of Variety of Pharmaceutical Compounds in High-pH Mobile Phases; Jian Wang; Mohammed Jemal; Bristol-Myers Squibb, Princeton, NJ
- WP 333 Development of a Desalting Interface for LC/MS

  Mobile Phase Containing Non-volatile Salts; Yutaka

  Takahashi 1,2; Kanae Teramoto 1; Kazumi Yoshida 3;
  Kazuhiro Chiba 3; JEOL, Tokyo, Japan; TUAT-TLO.

  Co. Ltd, Tokyo, Japan; Tokyo University of Agriculture and Technology, Tokyo, Japan
- WP 334 Reduce Column Related Carryover for Bioanalysis by Alternating the Column Flow Direction in LC/MS/MS; Susan Chen; Ji Zhang; Debra Liao; Michael Johnson; Shaoxia Yu; Justin Gordon; Jing-Tao Wu; Mark Qian; Millennium: The Takeda Oncology Company, Cambridge, MA
- WP 335 Novel Automated Online Column Switching HILIC-RP-LC/MS Method for the Analysis of Complex Samples; Egidijus Machtejevas<sup>1</sup>; Sven Andrecht<sup>1</sup>; Robertus Hendriks<sup>1</sup>; Klaus K. Unger<sup>2</sup>; <sup>1</sup>Merck KGaA, Darmstadt, Germany; <sup>2</sup>Johannes Gutenberg University, Mainz, Germany
- WP 336 A Novel Micro-Affinity Column for LC ICP-MS
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  Sabrina Tachdjian<sup>2</sup>; Naoki Furuta<sup>1</sup>; Kazunori Iwata<sup>3</sup>;
  Takashi Kotsuka<sup>3</sup>; <sup>1</sup>Chuo University, Tokyo, Japan;
  <sup>2</sup>Showa Denko America, Inc., New York, NY, <sup>3</sup>Showa Denko KK, Tokyo, Japan
- WP 337 Method Development Strategies for Ultra High-Throughput LC-MS/MS Analysis of Small Polar Molecules Utilizing HILIC Mechanisms; <u>Brian</u>

- Rappold; Russell Grant; Patricia Holland; Labcorp, Burlington, NC
- WP 338 Application of a Structured Approach for Method Development in Bioanalytical HILIC-MS/MS Applications; A. Carl Sanchez; Monika M. Kansal; Phenomenex, Torrance, CA
- WP 339 Identification and Separation of an Environmental Contaminant (Synephrine) During the Measurement of Free Phenylephrine in Human Plasma using ESI-HILIC-LC/MS/MS; Michael P. Waldron; Jordan Honrine; Patricia E. Paterson; Bruce Hidy; Rand G. Jenkins; PPD, Richmond, VA
- WP 340 Alternative LC Columns for Hydrophilic Compounds for Better Detection and Separation in LC/MS;

  <u>Kazuko Haseyama</u>; Hiroko Arai; Isao Yanagisawa;

  Taketoshi Kanda; Osamu Shirota; *Shiseido, Tokyo, Japan*
- WP 341 The Separation of Popular Cold, Sinus, and Allergy Medications using TSK-GEL ODS-140HTP Columns; Atis Chakrabarti; Shigeru Nakatani; J.Kevin O'Donnell; Tosoh Bioscienc LLC, Montgomerryville, PA
- WP 342 High Throughput Qualitative and Quantitative LC/MS Analyses Based on Fused-Core™
  Columns; Nelson Huang; Peter Tate; Ning Pan; Franklin Schlerman; Oliver McConnell; Wyeth, Cambridge, MA
- WP 343 Recent Advancements in Accelerated Bioanalytical LC/MS Using Fused-Core Columns; Richard L.

  Beardsley; Ethan R. Badman; Zhenmin Liang; Surendra Bansal; Hoffmann-La Roche Inc., Nutley, NJ
- WP 344 Evaluation of C18 Sub 2 Micron Particle Columns for UPLC Analysis of Drug-like Molecules; <u>Iris Scherer</u>; Melissa Gomez; Luke Miller; *GlaxoSmithKline*, *Rtp*, *NC*

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- WP 345 Sample Preparation of Phosphorus-Containing
  Amino Acid Herbicides Using TiO<sub>2</sub>-Coated
  Monolithic Spin Column; Shota Miyazaki; GL Sciences
  Inc., Saitama, Japan
- WP 347 In Preparative LC/MS, Loadability and Peak Shape Changes with pH and Concentration are Rationalized Based on Eluent Conditions and Analyte; Xu Zhang; Mark J. Hayward; Lundbeck Research USA, Paramus, NJ
- WP 347 Norbornene-Based Monolithic Pre-Columns for LC/MS Analysis in Nanomedical Research; Christina Gatschelhofer<sup>1</sup>; Agnes Mautner<sup>1</sup>; Michael R.
  Buchmeiser<sup>2</sup>; Andreas Zimmer<sup>3</sup>; Karin Wernig<sup>3</sup>; Thomas R. Pieber<sup>1,4</sup>; Frank M. Sinner<sup>1</sup>; Joanneum Research, Graz, Austria; Leibniz Institute for Surface Modification e.V., Leipzig, Germany; University of Graz, Graz, Austria; Medical University Graz, Graz, Austria
- WP 348 LC Autosampler with "Straight-to-Column"
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- WP 349 Automatic Non-Volatile Salt and Ion-Pair Reagent Removal System for Impurity Determination in Pharmaceutical Products; Satoshi Yamaki; Naoki Hamada; Yoshihiro Hayakawa; Shuzo Maruyama; Junko Iida; Shimadzu Corporation, Kanagawa, Japan
- WP 350 Automated Extraction of Pharmaceutical Compounds in Plasma; William Hudson; Yung-Lin Chen; Varian, Inc., Lake Forest, CA
- WP 351 Two Dimensional Online Solid-Phase Extraction Combined with Liquid Chromatography – Mass

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  Extraction with LC-MS/MS; Joseph Di Bussolo<sup>1</sup>; Rory
  Rohm<sup>2</sup>; <sup>1</sup>Thermo Fisher Scientific, West Chester, PA;
  <sup>2</sup>West Chester University of PA, West Chester, PA
- WP 353 Analysis of Melamine and Cyanuric Acid from Baby Formula with Clean Up Using Solid Phase Extraction (SPE); Shahana Huq; *Phenomenex, Torrance, CA*
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- WP 355 Understanding the Role of Oleic Acid and Its Metabolite in Atherosclerosis by Determining Their Levels in Human Plasma Using SPE-LC-MS/MS; Huiling Liu<sup>1</sup>; Qunjie Wang<sup>1</sup>; Changyong Xue<sup>2</sup>; Yinghua Liu<sup>2</sup>; Jin Wang<sup>2</sup>; Yuehong Zhang<sup>2</sup>; Xiaoxing Lv<sup>2</sup>; Junyan Zhang<sup>1</sup>; Jie Liao<sup>2</sup>; <sup>1</sup>Agela Technologies Inc, Newark, NJ; <sup>2</sup>General Hospital of Chinese PLA, Beijing, China
- WP 356 Impact of Side Reactions Involving Strong Cation Exchange SPE Mechanism on Bioanalytical Assay Accuracy by Using LC-MS/MS; Catherine Fontaine; Jean-Nicholas Mess; Milton Furtado; Fabio Garofolo; Algorithme Pharma Inc., Laval (Montreal), Quebec, CANADA
- WP 357 Modification of the QuEChERS Extraction
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  Laboratories, Hamilton, New Zealand; <sup>2</sup>University of
  Surrey, Guilford, UK
- WP 358 Analysis of Drugs of Abuse Using Automated
  Disposable Pipette Extraction and LC/MS/MS; Fred
  Foster<sup>1</sup>; William Brewer<sup>2</sup>; Sparkle Ellison<sup>2</sup>; Stephen
  Morgan<sup>2</sup>; Tom Gluodenis<sup>3</sup>; <sup>1</sup> Gerstel, Inc., Linthicum,
  MD; <sup>2</sup>University of South Carolina, Columbia, SC;
  <sup>3</sup>Agilent Technologies, Wilmington, DE
- WP 359 Multiresidue Analysis of Aminoglycoside Antibiotics
  Using Disposable Pipette Extraction and Liquid
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  Katerina Mastovska; Alan R. Lightfield; USDA-ARS-ERRC, Wyndmoor, PA

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- WP 360 Top Down Approaches for the Identification of Peptidic Toxins Containing Disulfide Bonds; Chafia Bennaceur<sup>1</sup>; Carlos Afonso<sup>1</sup>; Sandra Alves<sup>1</sup>; Anne Bossée<sup>2</sup>; Jean-Claude Tabet<sup>1</sup>; <sup>1</sup>Université Paris 6, Paris, France; <sup>2</sup>Centre d'Etudes du Bouchet, Vert-le-Petit, France
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  Using Different Tandem Mass Spectrometry
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  Mcluckey; Purdue University, West Lafavette, IN
- WP 362 Relevance of Peak Assignment Criteria in the Analysis of Disulfide-Bonded Peptides Using Collision Induced Dissociation Spectra; Daniel Clark; Melinda L Toumi; Eden P Go; Heather Desaire; University of Kansas, Lawrence, KS
- WP 363 Oxidative Cleavage of Disulfide Bond for Sequencing and Disulfide Mapping in Polypeptides; Yu Xia; R. Graham Cooks; Purdue Univeristy, West Lafayette, IN

- WP 364 ESI- and MALDI-MS/MS Analysis of Intramolecular Cross-Linked Peptides with a Photoactivated NHS-Diazirine Cross-linker; Alexandre F. Gomes; Fabio C Gozzo; Institute of Chemistry University of Campinas, Campinas, Brazil
- WP 365 Fragmentation of Intermolecular Cross-Linked
  Peptides by ECD and IRMPD; Luiz Fernando Arruda
  Santos; Amadeu H Iglesias; Fabio C Gozzo; IQ University of Campinas. Campinas. BRAZIL
- WP 366 TxXIIIA, an Atypical Homodimeric Conotoxin Found in the Conus textile Venom; Loic Quinton<sup>1</sup>; Nicolas Gilles<sup>2</sup>; Edwin De Pauw<sup>1</sup>; <sup>1</sup>University of Liege, Liège, Belgium; <sup>2</sup>CEA, iBiTec-S, SIMOPRO, Gif-sur-Yvette, France
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- WP 368 Characterization of Peptides from Skin Secretions of Amphibians by Composition-Based de novo Sequencing; Markus Langsdorf<sup>1</sup>; Alireza Ghassempour<sup>2</sup>; Andreas Roempp<sup>1</sup>; Bernhard Spengler<sup>1</sup>; 

  <sup>1</sup>Justus Liebig University, Giessen, Germany; <sup>2</sup>Shahid Beheshti University, Tehran, Iran
- WP 369 Sequencing of Peptides Produced in the Process of Mimicking Prebiotic Syntheses from Amino Acids by Thermocycling; Alexey Kononikhin<sup>1,3</sup>; Olga Demina<sup>3</sup>; Erast Kunenkov<sup>2</sup>; Andrey Khodonov<sup>3</sup>; Maria Indeykina<sup>2</sup>; Igor Popov<sup>1,3</sup>; Sergey Varfolomeev<sup>2,3</sup>; Eugene Nikolaev<sup>1,3</sup>; <sup>1</sup>The Institute for Energy Problems of Chemical Phys, Moscow, Russian Federation; <sup>2</sup>Lomonosov Moscow State University, Moscow, Russian Federation; <sup>3</sup>Emanuel Institute of Biochemical Physics, Moscow, Russian Federation
- WP 370 New Insights into Human Chromium Binding Peptides; Heather Watson; Yuan Chen; Carolyn J. Cassady; John B. Vincent; *University of Alabama*, Tuscaloosa, AL

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- WP 372 Natural Product Screening and Identification Using a Combination of High-throughput UPLC-TOF and Hybrid Linear Ion Trap FTMS LC/MS; Jeffrey R.

  Gilbert; Paul Lewer; Dennis O. Duebelbeis; Don R.
  Hahn; Dow AgroSciences, Indianapolis, IN
- WP 373 Mass Spectrometric Analysis of Polyketide Biosynthesis: Direct Infusion FTICR-MS Versus Low-Resolution LC-MS for Analysis of Active-Site Bound Intermediates; Christopher M Rath; David H Sherman; Kristina Hakansson; University of Michigan, Ann Arbor, MI
- WP 374 Structural Characterization of New Statin-Like Flavonoid Glycosides in Citrus Bergamia by High Resolution Mass Spectrometry; Leonardo Di Donna; Giuseppina De Luca; Anna Napoli; Fabio Mazzotti; Domenico Taverna; Giovanni Sindona; Università della Calabria, Dipartimento di Chimica, Arcavacata di rende (CS). Italy
- WP 375 High-Resolution TOF LC/MS Characterization of the Enzymatic Glycosylation of Stevia Rebaudiana: A Comparison of Natural and Enzyme-Treated Stevia

- Extracts; <u>Katrina Emmel</u><sup>1</sup>; Ted Waszkuc<sup>1</sup>; Susan Kraemer-Berkman<sup>1</sup>; Andre Szczesniewski<sup>2</sup>; Sue D'antonio<sup>2</sup>; <sup>1</sup>NOW Foods, Bloomingdale, IL; <sup>2</sup>Agilent Technologies, Schaumburg, IL
- WP 376 The Development of a New Algorithm for Empirical Formula Calculations Based On Multiple Molecular Ion Data; Ichiro Hirano<sup>1</sup>; Yusuke Inohana<sup>1</sup>; Yutaro Yamamura<sup>1</sup>; Norio Mukai<sup>1</sup>; Michizane Hashimoto<sup>2</sup>; Neil Loftus<sup>3</sup>; John Warrander<sup>3</sup>; <sup>1</sup>Shimadzu Corporation, Kyoto, Japan; <sup>2</sup>Astellas Pharma Inc., Tsukuba, Japan; <sup>3</sup>Shimadzu ISS, Manchester, UK
- WP 377 High Precision Molecular Formula Determinations of Phytochemicals in Plant Extracts using the Isotope Fine Structure obtained by 15T FT-ICR MS; Jang Mi Jin; Kyu Hwan Park; Dong Wan Lim; Jong Shin Yoo; Hyun Sik Kim; Korea Basic Science Institute, Daejon, South Korea
- WP 378 Characterization of Phenolic Compounds in Almond Agricultural Wastes by Negative Ion ESI LC/MS for Potential Nutraceutical Applications; Carina Minardi; Crisand Anderson; Anuradha Prakash; Christine A. Hughey; Chapman University, Orange, CA
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- WP 380 Determination of Cytotoxic Alkaloids in Houttuynia Cordata by Liquid Chromatography/Electrospray Ionization-Tandem Mass Spectrometry; Fang-Ju Chou; Ting-Ting Jong; Maw-Rong Lee; National Chung Hsing University, Taichung, Taiwan
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  Jing Dong<sup>1</sup>; Hashi Yuki<sup>1</sup>; Li Hongmei<sup>2</sup>; Ishimadzu
  Shanghai Office, Shanghai, China; National Institute of
  Metrology of China, Beijing, China
- WP 382 Use of GC-QTOF MS to Identify Unknown Compounds in Herbal Extracts; Viorica Lopez-Avila; Adrian P. Land; George Yefchak; Agilent Laboratories, Santa Clara, CA
- WP 383 Identification & Confirmation of Hydrolysable Tannins from Phyllagathis Preatermissa with Coupling of NMR & FTMS; Hooi Poay Tan<sup>1,2</sup>; Sui Kong Ling<sup>1</sup>; Cheng Hock Chuah<sup>2</sup>; Hun Teong Cheah<sup>3</sup>; 

  <sup>1</sup>Forest Research Institute Malaysia, Kepong, Selangor; 

  <sup>2</sup>University of Malaya, Kuala Lumpur, W.Persekutuan; 

  <sup>3</sup>Alpha Analytical Malaysia, Shah Alam, Malaysia
- WP 384 Tandem Mass Spectrometric Characterization of Echinomycin and Related Compounds; Takemichi Nakamura<sup>1</sup>; Kenji Watanabe<sup>2</sup>; Hiroki Oguri<sup>3</sup>; Hideaki Oikawa<sup>3</sup>; Hiroyuki Koshino<sup>1</sup>; <sup>1</sup>RIKEN, Wako, Japan; <sup>2</sup>Okayama University, Okayama, Japan; <sup>3</sup>Hokkaido University, Sapporo, Japan
- WP 385 A Shotgun Approach for Profiling Traditional Chinese Medicine Samples Using UPLC/TOF MSE Coupled with Multi-Variant Statistical Data Analysis; Kate Yu<sup>1</sup>; Baijping Ma<sup>2</sup>; John P. Shockcor<sup>1</sup>; Jose Castro-perez<sup>1</sup>; Heshui Yu<sup>2</sup>; Liping Kang<sup>2</sup>; Jie Zhang<sup>2</sup>; Yue Gao<sup>2</sup>; <sup>1</sup>Waters Corp, Milford, MA; <sup>2</sup>Beijing Institute of Radiation Medicine, Beijing, China

- WP 386 PCA Analysis of MS Spectroscopic Fingerprints to Differentiate Skullcap (Scutellaria lateriflora) from Germanders (Teucrium canadense, T. chamaedrys);

  Pei Chen¹; Fenhong Song²; James Harnly¹; Longze Lin¹;

  \*\*IUSDA, Beltsville, MD; \*\*2FDA, Lenexa, KS\*\*
- WP 387 Multidimensional Scaling (MDS) of Matrix Assisted Laser Desorption/Ionization Mass Spectra to Evaluate Hydrolysable Tannins and Anthocyanins;

  Rachael Leverence; Martha M. Vestling; Jess D. Reed;

  University of Wisconsin, Madison, WI
- WP 388 Microbial Volatile Organic Compounds of Aspergillus sp; Takae Takeuchi<sup>1,2</sup>; Haruna Tanaka<sup>2</sup>; Takahito Suzuki<sup>2</sup>; Shin-ich Iwaguchi<sup>2</sup>; Sachiyo Kaneko<sup>2</sup>; Masato Kiuchi<sup>1</sup>; Masako Iwamatsu<sup>1</sup>; Mamoru Okubo<sup>3</sup>; Takaomi Matsutani<sup>4</sup>; Yoshinori Hosokawa<sup>5</sup>; Yoshio Hashimoto<sup>6</sup>; Hajime Ishitani<sup>6</sup>; <sup>1</sup>National Institute of Advanced Industrial Science, Ikeda, Osaka, Japan; <sup>2</sup>Nara Women's University, Nara, JAPAN; <sup>3</sup>Soda Kogyo Co., Ltd., Higashi-Osaka, Japan; <sup>4</sup>Kinki University, Higashi-Osaka, Japan; <sup>5</sup>X-ray Precsision, Inc., Kyoto, Japan; <sup>6</sup>Shinnihondenko Co.Ltd., Osaka, Japan
- WP 389 Quantitation of Pterostilbene in Blueberrie Juice by Liquid Chromatography Electrospry Ionization Tandem Mass Spectrometry and Isotope Dilution; Fabio Mazzotti<sup>1</sup>; Hicham Benabdelkamel<sup>1</sup>; Bartolo Gabriele<sup>2</sup>; Leonardo Di Donna<sup>1</sup>; Anna Napoli<sup>1</sup>; Giovanni Sindona<sup>1</sup>; <sup>1</sup>Università della Calabria, Dipartimento di Chimica, Arcavacata Di Rende, ITALY; <sup>2</sup>Facolta' di Farmacia e Scienze della Nutrizione e, Rende, Italy
- WP 390 Analysis of the Skin Secretion of Odorrana
  Schmackeri, the Chinese Odorous Frog; Martijn
  Pinkse<sup>1</sup>; Geisa Caprini<sup>1</sup>; Tianbao Chen<sup>2</sup>; Chris Shaw<sup>2</sup>;
  Peter Verhaert<sup>1</sup>; \*\*Ipelft University of Technology, Delft,
  Netherlands; \*\*School of Pharmacy, Queen's University
  of Belfast, Belfast, UK
- WP 391 Direct Live Plant Molecular Analysis of Single Cell from Different Tissues; Mónica Lorenzo Tejedor;
   Hajime Mizuno; Naohiro Tsuyama; Takanori Harada;
   Tsutomu Masujima; Hiroshima Univ. BioMed.,
   Hiroshima, JAPAN
- WP 392 Elucidation of the Mass Fragmentation Processes of the Polyether Marine Toxins, Dinophysistoxins, with Isomer Discrimination using Sodiated Adduct Ions; Kevin James; Bebhine Carey; zuzana skrabakova; ambrose furey; Proteobio, Cork, Ireland

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- WP 393 Highly Efficient Phosphopeptide Enrichment Using TiO2 Coated Magnetic Beads: Phosphoproteomic Analysis of Drosophila Kc167 Cell Lysates; Lei Cheng¹; Sven Andrecht²; Joerg von Hagen²; Clause Juel Jensen³; Morten Frodin³; Ole N. Jensen¹; ¹Univ. of Southern Denmark, Odense, Denmark; ²Merck KGaA, Darmstadt, Germany; ³Biotech Research & Innovation Center, Copenhagen, Denmark
- WP 394 Development of PolyMAC-Ti, A Novel Soluble
  Nanopolymer-Based Phosphopeptide Enrichment
  Method; Anton Iliuk; Bethany Alicie; Vicky Martin;
  Robert Geahlen; Weiguo Andy Tao; Purdue University,
  West Lafayette, IN
- WP 395 **High Performance Phosphoproteomics Using Phase**Transfer Surfactant; <u>Takeshi Masuda</u><sup>1</sup>; Mio Iwasaki<sup>1,2</sup>;
  Yasuyuki Igarashi<sup>1</sup>; Masaru Tomita<sup>1,2</sup>; Yasushi
  Ishihama<sup>1,3</sup>; <sup>1</sup>Institute for Advanced Biosciences Keio
  University, Tsuruoka, Japan; <sup>2</sup>Keio University,
  Yamagata, Japan; <sup>3</sup>PRESTO, Japan Science and
  Technology Agency, Tokyo, Japan

- WP 396 A High-Throughput Analysis of Phosphopeptides
  Using a Biphasic Pre-Column; Tabiwang N. Arrey;
  Thorsten Wolfgang Jaskolla; Dominic Baemlisberger;
  Björn Meyer; Michael Karas; University of Frankfurt,
  Frankfurt Am Main, Germany
- WP 397 Enrichment of Phosphopeptides Using Polymer-Titanium(IV) Hybrid Materials on MALDI Plates; Wei-Han Wang; Yu-Jing Tan; Merlin L. Bruening; Michigan State University. East Lansing. MI
- WP 398 Direct on-TiO2 Isotopic Labeling of Phosphopeptides by iTRAQ – Qualitative and Quantitative Validation of TiO2 Phosphopeptide Enrichment Parameters; Martin R. Larsen; Univ. Southern Denmark, Odense, Denmark
- WP 399 A Screening Method for the Detection of Phosphorylated Peptides in High-Resolution Mass Spectra; Dirk Valkenborg<sup>1,2</sup>; Raf Van De Plas<sup>2</sup>; Rita Derua<sup>2</sup>; Etienne Waelkens<sup>2</sup>; Tomasz Burzykowski<sup>1</sup>; <sup>1</sup>UHasselt, Hasselt, Belgium; <sup>2</sup>K.U.Leuven, Leuven, Belgium
- WP 400 High Speed MALDI TOF/TOF Analysis Its
  Advantages for Identification of Digested Proteins
  and Screening for Phosphorylated Peptides in LCMSMS; <u>Dietmar Waidelich</u>; Christof E. Lenz; Dietrich
  Merkel; Matthias Glueckmann; Applied Biosystems,
  Darmstadt, Germany
- WP 401 Lys-N and Trypsin Cover Complementary Parts of the Phosphoproteome in a Refined SCX-Based Phosphoproteomics Approach; Shabaz Mohammed; Sharon Gauci; Andreas Helbig; Nadia Taouatas; A.f. Maarten Altelaar; Albert J.r. Heck; Utrecht University, Utrecht, Netherlands
- WP 402 Improved Sample Preparation for Phosphoproteome Analysis of Rat Brain Tissue; Erol E. Gulcicek; Kathryn L Stone; Can Bruce; Raimund I Herzog; Robert S Sherwin; Yale University, New Haven, CT
- WP 403 Application of Acid Hydrolysis on Bovine Beta-Casein to Investigate the Integral Phosphorylation; Jinhee Kim; Seongjae Shin; Hyo-jik Yang; Jeongkwon Kim; Chungnam National University, Daejeon, South Korea
- WP 404 The Determination of Flavin Binding to Rnf Family of Membrane Proteins by MALDI-MS/MS; Dmitri Zagorevski; Blanca Barquera; Rensselaer Polytechnic Institute, Trov. NY
- WP 405 Characterization of the Auto-Phosphorylation
  Mechanisms of an Oncogenic Fusion Protein NPMALK Using Tandem Affinity Purification-Mass
  Spectrometry; Peng Wang; Fang Wu; Leah C Young;
  Raymond Lai; Liang Li; University of Alberta,
  Edmonton, Canada
- WP 406 **Dun1 FHA Domain-Dependent Dun1 Phosphorylation by Mass Spectrometry**; Eric S.-W.

  <u>Chen</u><sup>1,2</sup>; Hyun Lee<sup>1</sup>; Ming-Daw Tsai<sup>1,2</sup>; <sup>1</sup> Genomic

  Research Center, Academia Sinica, Taipei, Taiwan;

  <sup>2</sup> National Taiwan University, Taipei, Taiwan
- WP 407 Regulation of Protein Phosphorylation at the Postsynaptic Density: Global Analysis Targeting Specific Kinase and Phosphatase Activities; Howard Jaffe<sup>2</sup>; Ayse Dosemeci<sup>1</sup>, <sup>1</sup>NINDS/NIH, Bethesda, MD; <sup>2</sup>NIH, NINDS, Gaithersburg, MD
- WP 408 LC-MS<sup>E</sup> Phosphopeptide Mapping of RhoA and RhoC following in vitro Phosphorylation by PKCε; Gregory S. Cavey<sup>1</sup>; Caryn L. Lehner<sup>1</sup>; Joan C. Krilich<sup>2</sup>; Quintin Pan<sup>3</sup>, <sup>1</sup>Van Andel Research Institute, Grand Rapids, MI; <sup>2</sup>Nanosphere Inc., Northbrook, IL; <sup>3</sup>Ohio

- State University Comprehensive Cancer Center, Columbus, OH
- WP 409 Identification of Protein Phosphorylation Sites of Human APPL1 Using MS, MS/MS, and IM-MS;

  Randi L. Gant -Branum; John A. Mclean; Vanderbilt University, Nashville, TN
- WP 410 Quantitative Cancer Stem Cell Phosphoprotein Profiling by Use of Tandem Mass Tags and LC-HCD-MS/MS in an LTQ-Orbitrap; Carol L. Nilsson<sup>6</sup>; Arugadoss Devakumar<sup>1</sup>; Roslyn Dillon<sup>1</sup>; John C. Rogers<sup>2</sup>; Bryan Krastins<sup>5</sup>; Mary Lopez<sup>5</sup>; Michael Rosenblatt<sup>3</sup>; Barbara Kaboord<sup>2</sup>; Charles A. Conrad<sup>4</sup>; 

  <sup>1</sup>Pfizer Global R & D, San Diego, CA; <sup>2</sup>ThermoFisher Scientific, Rockford, IL; <sup>3</sup>Thermo Scientific, Rockford, IL; <sup>4</sup>University of Texas, M.D.A.C.C., Houston, TX; 

  <sup>5</sup>Thermo Fisher Scientific, BRIMS Center, Cambridge, MA; <sup>6</sup>Pfizer Inc., San Diego, CA
- WP 411 **Temporal Analysis of Nocodazole-Induced Phosphorylation Using LTQ Orbitrap;** Kohji Nagano;
  Takashi Shinkawa; Hironori Mutoh; Osamu Kondoh;
  Sayuki Morimoto; Noriyuki Inomata; Motooki Ashihara;
  Nobuya Ishii; Yuko Aoki; <u>Masayuki Haramura</u>; *Chugai Pharmaceutical, Kamakura, Japan*
- WP 412 Phosphorylation of Arginine Guanidyl Groups as Posttranslational Protein Modificaiton; Andreas Schmidt<sup>2</sup>; Goran Mitulovie<sup>3</sup>; Jakob Fuhrmann<sup>1</sup>; Tim Clausen<sup>1</sup>; Karl Mechtler<sup>1,3</sup>; <sup>1</sup>IMP Research Institute of Mo, Vienna, Austria; <sup>2</sup>CD Laboratory / Vienna, Vienna, Austria; <sup>3</sup>IMBA Inst. of Mol. Biotech., Vienna, Austria
- WP 413 Mass Spectrometry Characterization of hCenexin1
  Phosphorylation Vital to Polo-like Kinase 1 (Plk1)
  Interaction for Mitotic Functions; Li-Rong Yu¹; Nak-Kyun Soung²; Jung-Eun Park²; Kyung H. Lee²; Jung-Min Lee³; Jeong K. Bang⁴; Timothy D. Veenstra⁵; Kunsoo Rhee³; Kyung S. Lee²; ¹National Center for Toxicological Research/FDA, Jefferson, AR; ²National Cancer Institute/NIH, Bethesda, MD; ³Seoul National University, Seoul, South Korea; ⁴Korea Basic Science Institute, Busan, South Korea; ⁵SAIC-Frederick, Inc., Frederick, MD
- WP 414 Label-Free Quantitation by LC-MS of the Global and Phosphoenriched Heart Tissue Proteome Reveals Novel Nitrite-Mediated Pathways to Cardioprotection; David H. Perlman; Giuseppe Infusini; Selena Bauer; Bernadette O. Fernandez; Vivek N. Bhatia; Mark E. Mccomb; Martin Feelisch; Catherine E. Costello; Boston University School of Medicine, Boston, MA

# PROTEIN CONFORMATION, 415 - 451

- WP 415 AMOM: Investigational New Analytical Marker of Oxidation for Monoclonal Antibodies using RP-LC/MS, Peptide Maps and SPR; John C. Le; Justin T. Paroski; Bernice Yeung; Byeong S. Chang; Symyx Technologies Inc., Camarillo, CA
- WP 416 Thermodynamic Measurements of Enzyme Stabilities
  Using H/D exchange and MALDI-TOF MS; ChengYing Lin; Yen-Peng Ho; National Dong Hwa
  University, Hualien, Taiwan
- WP 417 Ligand Binding to Cytochrome P450 46A1 as

  Assessed by Hydrogen Deuterium Exchange and
  Mass Spectrometry; Wei-Li Liao¹; Nathan Dodder²;
  Natalia Mast³; Irina A Pikuleva³; Illarion V. Turko¹;

  <sup>1</sup>Center for Advanced Research in Biotechnology,
  Rockville, MD; <sup>2</sup>NIST, Gaithersburg, MD; <sup>3</sup>Case
  Western Reserve University, Cleveland, OH

- WP 418 Allosteric Networks and Regulation of Protein Kinase A: Amide H/D Exchange Mass Spectrometry Reveals Parallels between cAMP Binding and Phosphorylation; Ganesh S. Anand<sup>1</sup>; Tanushree Bishnoi<sup>1</sup>; Susan Taylor<sup>2</sup>; Elizabeth Komives<sup>2</sup>; <sup>1</sup>National University of Singapore, Singapore, Singapore; <sup>2</sup>University of California, La Jolla, CA
- WP 419 **70S Ribosomal-Protein Dynamics in Translocation Revealed by H/D Exchange and Mass Spectrometry**;

  <u>Tatsuya Yamamoto<sup>1</sup></u>; Yoshihiro Shimizu<sup>2</sup>; Takuya
  Ueda<sup>2</sup>; Yoshitsugu Shiro<sup>1</sup>; <sup>1</sup>RIKEN, Sayo-gun, Japan;

  <sup>2</sup>Grad. Sch. Frontier Sci., Univ. Tokyo, Kashiwa, Japan
- WP 420 Two New Tools for Applying Chromatographic Retention Data to the Mass-Identification of HDX Peptides during HD-Exchange Experiments by NanoLC-MALDI; Enrique Cauich; Paul Gershon; UC-Irvine, Irvine, CA
- WP 421 Combined Ion Mobility and Rapid Gas-Phase
  Deuterium Labeling in a Synapt Mass Spectrometer
  for Enhanced Detection of Protein Conformations;
  Kasper D. Rand<sup>1</sup>; James P. Murphy III<sup>2</sup>; Keith Fadgen<sup>2</sup>;
  John R. Engen<sup>1</sup>; Northeastern University, Boston, MA;
  Waters Corporation, Milford, MA
- WP 422 Generation of Native Protein Ions and H/D Exchange in Liquid Sample Desorption Electrospray Ionization Mass Spectrometry (DESI-MS); Zhixin Miao; Hao Chen; Ohio University, Athens, OH
- WP 423 New Developments to HD Desktop Software for the Data Analysis of Hydrogen Exchange Mass Spectra;

  Bruce Pascal; Michael Chalmers; Jun Zhang; Scott
  Busby; Patrick R. Griffin; The Scripps Research
  Institute, Scripps Florida, Jupiter, FL
- WP 424 Characterization of Thermal Unfolding in Proteins
  Using Electrospray Ionization Time of Flight Mass
  Spectrometry and Top Down Fragmentation; Douglas
  Rehder; Sabine Paterson; David Hambly; Jaby Jacob;
  Michael J Treuheit; Bruce Kerwin; Himanshu Gadgil;
  Amgen Inc., Seattle, WA
- WP 425 IR Photodissociation Spectra of Gaseous Protein Ions: Hydrogen Bonding of Side-Chain Protonated Amino Groups is Unusually Strong; Xianglei Kong<sup>1</sup>; Kathrin Breuker<sup>2</sup>; Fred W. Mclafferty<sup>1</sup>; <sup>1</sup>Cornell University, Ithaca, NY; <sup>2</sup>University of Innsbruck, Innsbruck, Austria
- WP 426 New ECD Kinetic Probes of the Unfolding and Folding of Protein Conformers after Electrospray;

  Sergio Castro<sup>1</sup>; Kathrin Breuker<sup>2</sup>; Fred W. Mclafferty<sup>1</sup>;

  Cornell University, Ithaca, NY; <sup>2</sup>University of Innsbruck, Innsbruck, Austria
- WP 427 Fragmentation of of Gas Phase Ions of Ubiquitin Produced from Different Solution Conformations in a 3D Ion Trap; John Wright; Varian Inc., Wood Dale,
- WP 428 Mass spectrometry-Based Studies of the Vancomycin Resistance Pathway in Enterococcus faecalis;

  Charlotte A. Scarff, Andrew M. Quigley; Adrian J. Lloyd; David I. Roper; James H. Scrivens; University of Warwick, Coventry, UK
- WP 429 Development of Mass Spectrometry-Based
  Experimental Strategies for Detection and
  Characterization of Proteins with Non-Native
  Disulfide Bonds; Adriana Zeledon; Igor A. Kaltashov;
  University of Massachusetts, Amherst, MA
- WP 430 Computational Methods for Incorporation of Structural Mass Spectrometry Data in Structure Determination; Xiaojing Zheng<sup>1</sup>; Robert M Vernon<sup>2</sup>;

- David Baker<sup>2</sup>; Mark Chance<sup>3</sup>; <sup>1</sup>Case Western Reserve Univ., Cleveland, OH; <sup>2</sup>University of Washington, Seattle, WA; <sup>3</sup>Case Western Reserve Univers, Cleveland, OH
- WP 431 MS Cleavable Crosslinker for Protein Interactions; Billy Clifford-Nunn; Eric Simon; Philip Andrews; University of Michigan, Ann Arbor, MI
- WP 432 "MALDI-MS3" Analysis of CID-Cleavable
  Isotopically Coded Crosslinker TEABS; Jamie
  Thomas; Evgeniy Petrotchenko; Christoph Borchers;
  UVic-GBC Proteomics Centre, Victoria, Canada
- WP 433 Probing the Electrostatic Surface Topology of Proteins Using Combinatorial Collision-Induced Dissociative Chemical Crosslinking Reagents and Mass Spectrometry Analysis; Fan Liu; Michael B. Goshe; NC State University, Raleigh, NC
- WP 434 Structural Proteomics Revisited: A Top-Down
  Approach to Chemical Crosslinking and Protein
  Interactions; Giuseppe Infusini; Weiwei Tong; David
  H. Perlman; Roger Theberge; Catherine E. Costello;
  Boston University School of Medicine, Boston, MA
- WP 435 A Strategy for Efficient Identification of Chemically-Crosslinked Sites in Large Protein Complexes Using Label-Free LC-MS/MS Pattern Comparisons and Targeted MS/MS; Donghai Li<sup>1</sup>; Sandra L. Harper<sup>1</sup>; Hsin-yao Tang<sup>1</sup>; David W. Speicher<sup>1,2</sup>; <sup>1</sup>The Wistar Institute, Philadelphia, PA; <sup>2</sup>Wistar Institute, Philadelphia, PA
- WP 436 Development of Polyproline Linked Bifunctional Crosslinkers as Molecular Rulers for the Structural Investigation of Protein Assemblies; Timothy Garrett Jr.; Kevin B. Turner; Daniele Fabris; U. Maryland Baltimore County, Baltimore, MD
- WP 437 Structure Determination of Proteins from the Endoplasmic Reticulum Using Chemical Cross-Linking, Mass Spectrometry and Bioinformatics;

  Morten Rasmessen<sup>1</sup>; Tina Nielsen<sup>1</sup>; Gunnar Houen<sup>3</sup>; Juri Rappsilber<sup>2</sup>; Peter Hojrup<sup>1</sup>; <sup>1</sup>BMB, University of Southern Denmark, Odense M, Denmark; <sup>2</sup>Wellcome Trust Centre for Cell Biology, Edinburgh, UK; <sup>3</sup>Statens Serum Institut, Copenhagen, Denmark
- WP 438 Use of N-Terminal Modification with Isotopically
  Coded Reagents for Selective Identification of InterPeptide Crosslinks; Jason Serpa; Evgeniy Petrotchenko;
  Christoph Borchers; UVic-GBC Proteomics Centre,
  Victoria, Canada
- WP 439 Crosslinking Techniques for Structural Studies of Large, Multi-chain Coagulation-Related Proteins;

  Susan T. Lord<sup>1</sup>; Maria Warren Hines<sup>2</sup>; Evgeniy
  Petrotchenko<sup>3</sup>; Carol E. Parker<sup>2</sup>, <sup>1</sup>Department of
  Pathology & Lab.Medicine, UNC-CH, Chapel Hill, NC;
  <sup>2</sup>UNC-Duke Proteomics Center, UNC-CH, Chapel Hill,
  NC; <sup>3</sup>UVic-GBC Proteomics Centre, Victoria, BC
- WP 440 Out-gel Digest Procedure for Protein Cross-Linking Applications; Ashley Cabecinha; Evgeniy Petrotchenko; Christoph Borchers; UVic-GBC Proteomics Centre, Victoria. Canada
- WP 441 **Probability Based Shotgun Approach for Cross- Linking Sites Analysis by Mass Spectrometry**; Young
  Jin Lee; *Iowa State University, Ames, IA*
- WP 442 Characterization of β2m Dimer Formation using Covalent Labeling, Bottom-Up, and Top-Down Strategies; Vanessa Leah Mendoza<sup>1</sup>; Jonathan Wilson<sup>2</sup>; Desmond Kaplan<sup>2</sup>; Richard Vachet<sup>1</sup>; <sup>1</sup>University of Massachusetts, Amherst, MA; <sup>2</sup>Bruker Daltonics, Inc., Billerica, MA

- WP 443 Structural Study of C3b-H Complex Using Gamma and Synchrotron Irradiation Coupled with Semi-Quantitative Mass Spectrometry; Maxime Le Mignon<sup>1,2</sup>; Florence Gonnet<sup>1,2</sup>; Sebastien Brier<sup>1,2</sup>; Delphine Pflieger<sup>1,2</sup>; Bianca Sclavi<sup>3</sup>; Serge Pin<sup>4,5</sup>; Quentin Raffy<sup>4,5</sup>; Jean-Philippe Renault<sup>4,5</sup>; Régis Daniel<sup>1,2</sup>; <sup>1</sup>Université Evry-Val-d'Essonne, Evry, France; <sup>2</sup>CNRS UMR 8587, LAMBE, Evry, France; <sup>3</sup>CNRS UMR 8113, LBPA, Cachan, France; <sup>4</sup>CNRS URA 331 LCF, Gif-sur-Yvette, France; <sup>5</sup>CEA IRAMIS, Gif-sur-Yvette, France
- WP 444 **Probing the Structure of Proinsulin by MS-Based Footprinting**; <u>Janna Kiselar</u>; Nelson B. Phillips; Mark R
  Chance; Michael A. Weiss; *Case Western Reserve Univ*,
  Cleveland, OH
- WP 445 Computational Methods for Examining Covalently
  Labeled Biomolecules Using Structural Mass
  Spectrometry; Parminder Kaur; Janna Kiselar; Mark
  Chance; Case Western Reserve University, Cleveland,
  OH
- WP 446 Characterizing the ATP-Induced Structural Changes of the N-Terminal Domain of Pms1 by Oxidative Surface Mapping and Mass Spectrometry; Allison N Schorzman<sup>1</sup>; Lalith Perera<sup>1</sup>; Lars C. Pedersen<sup>1</sup>; Jenny M. Cutalo<sup>2</sup>; Thomas A. Darden<sup>1</sup>; Thomas A. Kunkel<sup>1</sup>; Kenneth B. Tomer<sup>1</sup>; \*\*INIEHS, RTP, NC; \*\*2FBI, Washington, D.C., DC
- WP 447 Autoantigen Structural Studies: Photolytic Oxidation and Chemical Modification Combined with Mass Spectrometry; Jinglan Wang; James G Smedley III; Piotr J Bilski; Jeffrey F Kuhn; Kenneth B. Tomer; Leesa Deterding; NIEHS, Research Triangle Park, NC
- WP 448 Laser-Induced Oxidative Labeling of Proteins for Probing Folding Kinetics and Mechanisms; Bradley B. Stocks; Lars Konermann; Univ. of Western Ontario, London, Canada
- WP 449 Structural Characterization of an Integral
  Membrane Protein by Oxidative Methionine
  Labeling and Mass Spectrometry; Yan Pan; Uni. of
  Western Ontario, London, Canada
- WP 450 High Sensitivity Characterization of Conformational Differences in Pharmaceutical Proteins by Rapid Hydroxyl Radical Footprinting; Caroline Watson<sup>1</sup>; Sergio G Tisminetzky<sup>2</sup>; Marshall W. Bern<sup>3</sup>; Joshua S. Sharp<sup>1</sup>; <sup>1</sup>Complex Carbohydrate Research Center/UGA, Athens, GA; <sup>2</sup>Biotechnology Development Group, ICGEB, Trieste, Italy; <sup>3</sup>Palo Alto Research Center, Palo Alto, CA
- WP 451 MS-based Carboxyl Group Protein Footprinting for Probing the Orientation of FMO Protein in Photosynthetic Bacterial Membranes; Hao Zhang; Jianzhong Wen; Robert E. Blankenship; Michael L. Gross; Washington University, Saint Louis, MO

# **NON-COVALENT INTERACTIONS, 452 - 464**

- WP 452 Investigation of Protein-Protein Complex
  Noncovalent Interactions by Quadrupole, Ion
  Mobility Separation Time-of-Flight Mass
  Spectrometry; Sheng Zhang<sup>1</sup>; Abiola Pollard<sup>1</sup>; Michael
  Daly<sup>2</sup>; Brian Crane<sup>1</sup>; \*\*Cornell University, Ithaca, NY;
  \*\*Waters Corp, Oakland, CA\*\*
- WP 453 Determining Stoichiometry of Noncovalent Protein Complexes using LC-MS/MS Label-Free Protein Quantification; Shirley H. Lomeli; Pinmanee Boontheung; Joseph A. Loo; UCLA, Los Angeles, CA
- WP 454 Towards the Elucidation of the Protein Complexes
  Involved in Prokaryotic Origin Independent DNA

- **Replication Restart An ESI-MS Study**; <u>Lindsey Easthon</u>; Jingshu Guo; Timothy Mueser; Wendell P. Griffith; *University of Toledo, Toledo, OH*
- WP 455 Antibody / Antigen Complexes: Characterization of Immune Complexes Using Noncovalent Mass Spectrometry; Cédric Atmanene<sup>1</sup>; Elsa Wagner-Rousset<sup>2</sup>; Nathalie Corvaia<sup>2</sup>; Alain Van Dorsselaer<sup>1</sup>; Alain Beck<sup>2</sup>; Sarah Sanglier-Cianferani<sup>1</sup>; <sup>1</sup>CNRS IPHC University of Strasbourg, Strasbourg, France; <sup>2</sup>Centre d'Immunologie Pierre Fabre, Saint-Julien-en-Genevois, France
- WP 456 Optimization of Hydroxyl Radical Surface Mapping Method Combined with Molecular Dynamics Simulations for Characterizing Macromolecular Interactions; Olga Charvatova<sup>1</sup>; Daniel Nesbitt<sup>1</sup>; Marshall W. Bern<sup>2</sup>; Joshua S. Sharp<sup>1</sup>; Ron Orlando<sup>1</sup>; Robert J. Woods<sup>1</sup>; <sup>1</sup>University of Georgia, Athens, GA; <sup>2</sup>Palo Alto Research Center, Palo Alto, CA
- WP 457 **Protein Aggregates: Fast Semi-Quantitation Analysis by High-Mass MALDI ToF Analysis**; <u>Alexis Nazabal</u>;
  Marc Dodeller; Nathalie Riesen; Benoit Plet; Ryan
  Wenzel; *CovalX AG, Zürich, Switzerland*
- WP 458 CLIP: A Crosslinker for Enrichment and Confident Identification of Protein Crosslinking Sites by Mass Spectrometry; Saiful M. Chowdhury<sup>1</sup>; Xiuxia Du<sup>2</sup>; Nikola Tolic<sup>1</sup>; Ashoka D. Polpitiya<sup>1</sup>; Ronald J. Moore<sup>1</sup>; John R. Cort<sup>1,3</sup>; Uljana M. Mayer<sup>1</sup>; Richard D. Smith<sup>1</sup>; Joshua N. Adkins<sup>1</sup>; \*\*IPacific Northwest National Laboratory, Richland, WA; \*\*2University of North Carolina, Charlotte, NC; \*\*3Washington State University, Tri-cities, Richland, WA
- WP 459 Technology Development for Studying Transient
  Protein-Protein Interactions on Chromosomes:
  Identification of a Transient Acetyltransferase
  Interactome; Samuel G. Mackintosh<sup>1</sup>; Sherri K. Smart<sup>1</sup>;
  Sean D. Taverna<sup>2</sup>; Ricky D. Edmondson<sup>1</sup>; Alan J.
  Tackett<sup>1</sup>; <sup>1</sup>University of Arkansas for Medical Sciences,
  Little Rock, AR; <sup>2</sup>Johns Hopkins Medical School,
  Baltimore, MD
- WP 460 Structural Characterization of Macromolecular Protein Complexes Using Chemical Cross-Linking and Mass Spectrometry; Pragya Singh; Richard A. Pfuetzner; Scott A. Shaffer; Alexandre Panchaud; Eri Nakatani; Carlos E. Catalano; Samuel I. Miller; David R. Goodlett; University of Washington, Seattle, WA
- WP 461 **Defining Topological Features of Membrane Proteins by Electrospray Ionization Mass Spectrometry**;

  <u>Lynsey N. Jones</u>; Stephen A. Baldwin; Peter J. F.

  Henderson; Alison E. Ashcroft; Astbury Centre for

  Structural Molecular Biology, University of Leeds,

  Leeds, UK
- WP 462 Photo-Crosslinking and Complementary Use of ESI and MALDI Mass Spectrometry to Map Interaction Sites between Transcriptional Activators and Mediator 15; Bo Wang; Chinmay Majmudar; Anna Mapp; Kristina Hakansson; University of Michigan, Ann Arbor, MI
- WP 463 An Integrative Proteomic Approach to Identify Huntingtin Protein Networks Using a Novel BAC Transgenic Model of Huntington's Disease; Dyna I. Shirasaki<sup>1</sup>; Erin R. Greiner<sup>1</sup>; Pinmanee Boontheung<sup>1</sup>; Steve Horvath<sup>2</sup>; X. William Yang<sup>3</sup>; Joseph A. Loo<sup>1</sup>; 

  <sup>1</sup>UCLA, Department of Chemistry and Biochemistry, Los Angeles, CA; <sup>2</sup>UCLA, Department of Biostatistics, Los Angeles, CA; <sup>3</sup>UCLA, Brain Research Institute, Los Angeles, CA

WP 464 Characterization of Protein Complexes from Human Pancreatic Cancer Cell Using a Combination of Native-PAGE and Mass Spectrometry; Xinli Wang; Guoqiang Chen; Zhiyun Zhao; Zhili Li; Institute of Basic Medical Sciences, CAMS & PUMC, Beijing, China

# CARBOHYDRATE / OLIGOSACCHARIDES, 465 - 491

- WP 465 A Comprehensive Method for Separating Neutral, Sialylated, and Sulfated N-linked Glycans in Their Native and Permethylated Forms; Sergei Snovida; Ed Bodnar; Helene Perreault; University of Manitoba, Winnipeg, Canada
- WP 466 Profiling and Quantitation of Recombinant
  Monoclonal Antibody Glycosylation by NanoLC/ESI-MS with the On-Chip Deglycosylation:
  Comparison to MALDI-TOF MS and CE-LIF;
  Tomasz K. Baginski<sup>1</sup>; Maggie Bynum<sup>2</sup>; Rodney Keck<sup>1</sup>;

  Genentech, Inc., South San Francisco, CA; <sup>2</sup>Agilent
  Technologies, Santa Clara, CA
- WP 467 An LC/MS Platform for Aminated Oligosaccharide
  Analysis in Both Positive and Negative Modes:
  towards More Complete Structural Assignment; Ewa
  Jankowska; John F Cipollo; Food and Drug
  Administration CBER, Bethesda, MD
- WP 468 Characterization of Complex N-Glycans Using High pH Anion Exchange and in-line Mass Spectrometry (HPAEC/MS); Louise Chen; Bhavana Shah; Gary Rogers; Amgen, Thousand Oaks, CA
- WP 469 N-glycans Profiling Using Capillary Liquid
  Chromatography and High Mass Accuracy
  Electrospray Mass Spectrometry: Application to the
  Characterization of Therapeutic Glycoproteins;
  Valegh Faid; Magali Andre; Nicolas Bihoreau;
  Guillaume Chevreux; LFB, Courtaboeuf, France
- WP 470 An Integrated Microfluidic LC/MS Chip Workflow for Rapid On-line Deglycosylation and Characterization of N-glycans from IgG Antibodies; Maggie A. Bynum<sup>1</sup>; Hongfeng Yin<sup>1</sup>; Katie Felts<sup>2</sup>; Yvonne Lee<sup>2</sup>; Craig Monell<sup>2</sup>; Kevin Killeen<sup>1</sup>; <sup>1</sup>Agilent Laboratories, Santa Clara, CA; <sup>2</sup>Agilent Technologies, La Jolla, CA
- WP 471 Profiling and Characterization of N- and O-Linked Glycans Released from Glycoproteins Using RP-HPLC with Charged Aerosol Detection and Mass Spectrometry; Andrew Hanneman; Jason Rouse; Wyeth BioPharma, Andover, MA
- WP 472 High Resolution CE-MS Separation of APTS-Labeled Glycans; Tomas Rejtar; Dipak Thakur; Zhenke Liu; Andras Guttman; Barry L. Karger; Northeastern University, Boston, MA
- WP 473 Structure Library for Oligosaccharides Built on Retention Times and Accurate Masses; Shuai Wu<sup>1</sup>; Nannan Tao<sup>1</sup>; J. B. German<sup>1</sup>; Rudi Grimm<sup>2</sup>; Carlito B. Lebrilla<sup>1</sup>; <sup>1</sup>UC Davis, Davis, CA; <sup>2</sup>Agilent Technologies, Palo Alto, California
- WP 474 Combining Fully Automated Chip-Nanoelectrospray Ion Trap Mass Spectrometry and GanglioSoft 1.2 Computer Software for Identification of Human Hemangioma Gangliosides; Catalin C. Schiopu<sup>1</sup>; Alina F. Serb<sup>2</sup>; Eugen Sisu<sup>2</sup>; Zeljka Vukelic<sup>3</sup>; Alina D. Zamfīr<sup>4</sup>; <sup>1</sup>National Institute for R&D in Electrochemistry, Timisoara, Romania; <sup>2</sup>University of Medicine and Pharmacy, Timisoara, Romania; <sup>3</sup>University of Zagreb, Zagreb, Croatia; <sup>4</sup>University Aurel Vlaicu Arad, Arad, Romania

- WP 475 **Software Utilities for Automated Glycomics**; <u>Sergey Y. Vakhrushev</u>; Denis Dadimov; Jasna Peter-Katalinic; Institute of Medical Phys, Muenster, Germany
- WP 476 Can a Peptide Map Replace The Traditional Glycan Map for N-Glycan Analysis? Bhavana Shah; Xinzhao Grace Jiang; Louise Chen; Zhongqi Zhang; Amgen, Inc., Thousand Oaks, CA
- WP 477 Multiple Reaction Monitoring Liquid
  Chromatography Mass Spectrometry for
  Monosaccharide Compositional Analysis of
  Glycoproteins; Loubna A. Hammad; Marwa Saleh;
  Milos V. Novotny; Yehia Mechref; Indiana University
  Biochem Ctr, Bloomington, IN
- WP 478 Optimization of Three Atmospheric Pressure Mass Spectrometry (AP-MS) Techniques to Observe Oligosaccharide Degradation Products in Naturally and Artificially Aged Paper; Catherine H. Stephens<sup>1,2</sup>; Bindesh Shrestha<sup>3</sup>; Paul M. Whitmore<sup>1,2</sup>; Mark E. Bier<sup>2</sup>; Akos Vertes<sup>3</sup>; <sup>1</sup>Art Conservation Research Center, Pittsburgh, PA; <sup>2</sup>Carnegie Mellon University, Pittsburgh, PA; <sup>3</sup>George Washington University, Washington, DC
- WP 479 Differentiation of Lithium Cation-Attached Monoand Disaccharide Isomers by Wavelength-Dependent CO<sub>2</sub> Laser Photofragmentation and FTICR Mass Spectrometry; John R. Eyler; Sarah E. Stefan; University of Florida, Gainesville, FL
- WP 480 Structural Characterization of 1-octyl-β-D-Glucopyranoside Using Zinc Cationization. An Electrospray Ionization and Tandem Mass Spectrometry Study; Khaled Edbey¹; Grainne Moran²; Gary Willett²; ¹University of Garyounis, Benghazi, Libya; ²The University of New South Wales, Sydney, NSW
- WP 481 Changes in Modifications of Cell Wall
  Oligosaccharides from Lignocellulosic Biomass
  During AFEX Pretreatment Using LC/TOFMS and
  Multiplexed CID; Ramin Vismeh; Shishir P
  Chundawat; Venkatesh Balan; Bruce E Dale; A. Daniel
  Jones; Michigan State University, East Lansing, MI
- WP 482 Infrared Multiple Photon Dissociation (IRMPD)
  Spectra of Rubidium Cation-Tagged D-Glucuronic
  and L-Iduronic Acids; Emilio Cagmat; Jan
  Szczepanski; Nicolas Polfer; David H. Powell; John R.
  Eyler; Department of Chemistry, University of Florida,
  Gainesville, FL
- WP 483 Compositional and Structural Analysis of
  Gangliosides in Human Cerebrospinal Fluid by ChipBased Nanoelectrospray Ionization Tandem Mass
  Spectrometry; Alina F. Serb¹; Catalin C. Schiopu²;
  Dragana Marincic³; Zeljka Vukelic³; Alina D. Zamfir⁴;
  ¹University of Medicine and Pharmacy, Timisoara,
  Romania; ²National Institute for R&D in
  Electrochemistry, Timisoara, Romania; ³University of
  Zagreb, Zagreb, Croatia; ⁴Aurel Vlaicu University of
  Arad, Arad, Romania
- WP 484 Characterization of Protein Glycosylation
  Intermediates by LC-MS/MS on Porous Graphitic
  Carbon: Discovery of C45 and C60 PolyisoprenylOligosaccharide Lipid Carriers; Jacek Stupak<sup>1</sup>;
  Christopher Reid<sup>1</sup>; Christine M. Szymanski<sup>2</sup>; Jianjun Li<sup>1</sup>;

  \*\*National Research Council, Ottawa, ON; \*\*2AICCS,
  University of Alberta, Edmonton, AB
- WP 485 MALDI Tandem MS Analysis of Cellulose and Related Biomolecules: Potential for MS Imaging of

- Cellulosic Tissues; Kyle A. Lunsford; Gary F. Peter; Richard A. Yost; *University of Florida, Gainesville, FL*
- WP 486 Analysis of Mycothiol and Mycothione Levels from Wild-Type and mtr Mutant Strains from Mycobacterium smegmatis; Cynthia M Holsclaw<sup>1</sup>; Wilson B Muse<sup>3</sup>; Kate Carroll<sup>3</sup>; Julie A. Leary<sup>1,2</sup>; 

  <sup>1</sup>Section of MCB, University of California, Davis, CA; 
  <sup>2</sup>Department of Chemistry, University of California, Davis, CA; 
  <sup>3</sup>Life Sciences Institute, University of Michigan, Ann Arbor, MI
- WP 487 Analysis of Brain Chondroitin/Dermatan Sulfate Glycosaminoglycans by Fully Automated Chip-Based Nanoelectrospray Multistage Mass Spectrometry;

  Corina Flangea<sup>2</sup>; Eugen Sisu<sup>2</sup>; Daniela Seidler<sup>3</sup>; Alina D. Zamfir<sup>1</sup>, <sup>1</sup>University Aurel Vlaicu Arad, Arad, Romania; <sup>2</sup>University of Medicine and Pharmacy, Timisoara, Romania; <sup>3</sup>University of Muenster, Muenster, Germany
- WP 488 Strategies toward Characterizing Sulfated Glycans in Recombinant Proteins; John J. Thomas<sup>1</sup>; Paul Salinas<sup>1</sup>; Gregory O Staples<sup>2</sup>; Hicham Naimy<sup>2</sup>; Joseph Zaia<sup>2</sup>; Philip J. Savickas<sup>1</sup>; <sup>1</sup>Shire HGT, Cambridge, MA; <sup>2</sup>Boston University School of Medicine, Boston, MA
- WP 489 The Occurrence of Rare, Unsubstituted
  Glucosamine-Containing Disaccharides in Heparan
  Sulfate from Bovine and Rat Tissues: an SEC LC/MS
  Study; Xiaofeng Shi; Joseph Zaia; Boston University
  School of Medicine, Boston, MA
- WP 490 On-Line Tandem Mass Spectrometry for Characterization of Protein Binding Heparan Sulfate Octasaccharides; Hicham Naimy; Nancy Leymarie; Joseph Zaia; Boston University School of Medicine, Boston. MA
- WP 491 Improved HILIC LC/MS Analysis of Heparinoids
  Using a Chip with Post-column Make-Up Flow;
  Gregory O. Staples<sup>1</sup>; Hicham Naimy<sup>1</sup>; Hongfeng Yin<sup>2</sup>;
  Karsten Kraiczek<sup>3</sup>; Kevin Killeen<sup>2</sup>; Catherine E.
  Costello<sup>1</sup>; Joseph Zaia<sup>1</sup>; \*\*IBoston University School of Medicine, Boston, MA; \*\*2Agilent Laboratories, Santa Clara, CA; \*\*3Agilent Technologies, Waldbronn, Germany

# PROTEINS, GLYCOPROTEINS, 492 - 512

- WP 492 Biological Activities and Compositions of Protein Extracted from Kaempferia Parviflora Wall. Ex. Baker; Polkit Sangvanich; Chuklalongkorn University, Bangkok, Thailand
- WP 493 Characterization of the Disulfide Connectivity and Nlinked Glycosylation of KLH using a LTQ with CID and ETD; Justin B. Sperry; Halyna E. Narepekha; Qin Zou; James A. Carroll; Pfizer, Saint Louis, MO
- WP 494 A Novel Approach for Identification and Quantitation of Protein Glycosylation Pattern by Precursor Ion Scan and H-SRM on QQQ Instrument; Andreas F.R Hühmer<sup>1</sup>; Reiko Kiyonami<sup>1</sup>; Shiaw-lin Wu<sup>2</sup>; Barry L. Karger<sup>2</sup>; Vlad Zabrouskov<sup>1</sup>; William S. Hancock<sup>2</sup>; <sup>1</sup>ThermoFisher Scientific, San Jose, CA; <sup>2</sup>Barnett Institute, Northeastern University, Boston, MA
- WP 495 Electron Capture Dissociation of Sialated Glycopeptides; Prasanna Ramachandran; Sheng Yin; Rachel R Ogorzalek Loo; Joseph A. Loo; University of California,, Los Angeles, CA
- WP 496 Parallel Structural Characterization of Glycopeptides and Glycoprotein Quantification by Electrospray Quadrupole Ion-Mobility Time-of-Flight Mass Spectrometry with Ultra Performance Liquid Chromatography; Hui Wei<sup>1</sup>; Wen Ding<sup>2</sup>; John

- Kelly<sup>2</sup>, <sup>1</sup>Waters Corporation, Milford, MA; <sup>2</sup>National Research Council of Canada, Ottawa, Ontario, Canada WP 497 Combined Analysis Of Protein Glycosylation and Label-Free-Glycoprotein-Bacteria Interactions Using
  - MALDI-FTICR MS and Scanning Optical
    Microscope Based on OI-RD; Mariana Barboza; Yiyan
    Fei; David A. Mills; Bruce J. German; XiangDong Zhu;
    Carlito Lebrilla; University of California,, Davis, CA
- WP 498 Analysis of Site-Specific Glycosylation Profile of Glycoproteins by LC-ECD-MS/MS in a Radio Frequency Linear Ion Trap; Takeshi Sakamoto; Naomi Manri; Hiroyuki Satake; Akihito Kaneko; Central Res. Lab., Hitachi, Ltd., Tokyo, Japan
- WP 499 Site-Specific Glycoprofiling of N-Linked Glycopeptides Using MALDI-TOF MS; Morten Thaysen-Andersen; Simon Mysling; Peter Hojrup; BMB, University of Southern Denmark, Odense M, Denmark
- WP 500 Application of Source CID MS/MS Scan with Combination of CID and PQD Fragmentations to Rapidly Identify and Characterize Glycoproteins; Yite Chou; Amgen, Thousand Oaks, CA
- WP 501 A Glycoproteomics Approach for Profiling of Pharmaceutical Compounds Using Quantitative Glycopeptide Enrichment and Online LC (HILIC/RP) Mass Spectrometry; Jessica Wohlgemuth; Thomas Eichhorn; Robertus Hendriks; Sven Andrecht; Merck KGaA, Darmstadt, Germany
- WP 502 Comprehensive Characterization of Haptoglobin Glycosylation Using a PLOT LC column with a Thermo LTQ-ETD-MS; Dongdong Wang; Marina Hincapie; Shiaw-Lin Wu; Barry L. Karger; Northeastern University, Boston, MA
- WP 503 Assigning the Glycosylation Sites of Glycoproteins
  Using Endo-M in Conjunction with LC/MSMS;

  Ahmed Hussein<sup>1,2</sup>; Zaneer, M. Segu<sup>1,3</sup>; Milos, V.
  Novotny<sup>1,2</sup>; Yehia Mechref<sup>1,2</sup>; <sup>1</sup>Dept of Chemistry,
  Indiana University, Bloomington, IN; <sup>2</sup>National Center
  for glycomics and glycoproteomics, Bloomington, IN;

  <sup>3</sup>METACyt Biochemical Analysis Center, Bloomington,
  IN
- WP 504 Identification and Quantitation of Sialylated glycopeptides as Cancer Biomarkers Using TiO2 Chromatography Combined with iTRAQ, O18-Labeling and MRM; Sara Eun Lendal 1.2; Søren Cold3; Martin R. Larsen2; Protein Research Group, Odense, Denmark; Univ. Southern Denmark, Odense, Denmark; Odense University Hospital, Odense, Denmark
- WP 505 Identification and Quantification of Glycoproteins
  Using Ion-Pairing Normal-Phase Liquid
  Chromatography and Mass Spectrometry; Wen
  Ding<sup>1</sup>; Harald Nothaft<sup>2</sup>; Christine Szymanski<sup>2</sup>; John F.
  Kelly<sup>1</sup>; <sup>1</sup>National Research Council of Canada, Ottawa,
  ON; <sup>2</sup>University of Alberta, Edmonton, AB
- WP 506 Method Optimization for the Determination of Protein Site of N-Glycosylation: Case Study for SynCAM 1; Edward Voss<sup>1</sup>; Thomas Biederer<sup>1</sup>; Terence Wu<sup>1</sup>; Michael L. Easterling<sup>2</sup>; Mary LoPresti<sup>1</sup>; Kenneth R. Williams<sup>1</sup>; Tukiet T. Lam<sup>1</sup>; <sup>1</sup>Yale University, New Haven, CT: <sup>2</sup>Bruker Daltonic, Billerica, MA
- WP 507 Pancreatic Cancer Serum Detection Using A
  Lectin/Glyco-Antibody Array Method; Chen Li<sup>1</sup>;
  Eugene Zolotarevsky<sup>1</sup>; Michelle A. Anderson<sup>1</sup>; Dean E.
  Brenner<sup>1</sup>; Diane M. Simeone<sup>1</sup>; David M. Lubman<sup>1</sup>; Fan
  Xiang<sup>2</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI;
  <sup>2</sup>Shimadzu Biotech, Pleasanton, CA

- WP 508 A Novel Enrichment Method for Analysis of Sulfated Glycopeptides with MALDI TOF MS; Masaaki
  Toyoda; Hisashi Narimatsu; Akihiko Kameyama;
  Research Center for Medical Glycoscience, AIST,
  Tsukuba, Ibaraki, Japan
- WP 509 Glycoprotein Capturing through Functionalized Magnetic Nanoparticles; Hyo-jik Yang¹; Seongjae Shin¹; Eun Hye Park¹; Jinhee Kim¹; Yangsun Kim²; Jeongkwon Kim¹; ¹Chungnam National University, Daejeon, South Korea; ²Hudson Surface Technology, Newark, NJ
- WP 510 Highly Sensitive MALDI-MS<sup>n</sup> for Identification of Glycopeptides by a Simple Pyrene-Derivatization Method; Junko Amano; Takashi Nishikaze; Fumio Tougasaki; *The Noguchi Institute, Itabashi, Japan*
- WP 511 Enrichment and Identification of Glycoproteins and Glycan Using Nano-Scale Chelating Con A Monolithic Capillary; Shun Feng<sup>1</sup>; Na Yang<sup>1</sup>; Subramaniam Pennathur<sup>1</sup>; Steve Goodison<sup>2</sup>; David M. Lubman<sup>1</sup>; Fan Xiang<sup>3</sup>; <sup>1</sup>University of Michigan, Ann Arbor, MI; <sup>2</sup>University of Florida, Jacksonville, FL; <sup>3</sup>Shimadzu Biotech, Pleasanton, CA
- WP 512 A Comparison Study of Glycopeptides Enrichment of Boronic Acid Derived Magnetic Beads and Bare Silica-Coated Magnetic Nanoparticles; Ming-yi Ho; Chung-lin Liao; Academia Sinica, Taipei, Taiwan

#### PLASMA PROTEOMICS, 513 - 524

- WP 513 Method for Purification and Identification of Protein Biomarker from Human Serum Using TOF-TOF Instrument; Vanitha Thulasiraman<sup>1</sup>; Matthew Hammond<sup>1</sup>; Amanda Bulman<sup>1</sup>; Steve Roth<sup>1</sup>; Mariana Rusa<sup>1</sup>; Enrique Dalmasso<sup>1</sup>; Diane Mccarthy<sup>2</sup>; Fiona Plows<sup>3</sup>; \*\*IBio-Rad Laboratories, San Jose, CA; \*\*2Bio-Rad, Malvern, PA; \*\*3Bio-Rad Laboratories, Inc., Hercules, CA
- WP 514 Quantitative Analysis of Chaotropic & Solvent
  Effects on the Trypsin Digestion Efficiency of Human
  Plasma; Michael A. Kuzyk<sup>1</sup>; <u>Darryl Hardie</u><sup>1</sup>; Juncong
  Yang<sup>1</sup>; Derek Smith<sup>1</sup>; Angela M. Jackson<sup>1</sup>; N. Leigh
  Anderson<sup>2</sup>; Jennifer Proc<sup>1</sup>; Christoph H. Borchers<sup>1</sup>;

  \*\*IUVic-Genome BC Proteomics Centre, Victoria,
  Canada; \*\*Plasma Proteome Institute, Washington, D.C.\*\*
- WP 515 Analysis of Native Proteins by NanoLC-FT-ICR-MS: Application to the Identification of Apoliprotein A-I Modifications Induced by Oxidative Stress; Alexia Ortiz<sup>1</sup>; Gérald Luc<sup>2</sup>; Caroline Tokarski<sup>1</sup>; Christian Rolando<sup>1</sup>; <sup>1</sup>Univ. des Science/Tech de Lille, Villeneuve d'Ascq, France; <sup>2</sup>Université du Droit et de la Santé, Lille, France
- WP 516 Changes in the Maternal Serum Proteome between the 1st and 3rd Trimesters of Uncomplicated Pregnancy in Nepal; Peter Scholl<sup>1,3</sup>; Marjan Gucek<sup>2</sup>; Roberto Diez<sup>2</sup>; Ingo Ruczinski<sup>3</sup>; Alissa Rennie<sup>3</sup>; Chris Nathasingh<sup>3</sup>; Robert N. Cole<sup>2</sup>; James Yager<sup>3</sup>; John D. Groopman<sup>3</sup>; Kerry Schulze<sup>3</sup>; Parul Christian<sup>3</sup>; Keith West<sup>3</sup>; <sup>1</sup>US FDA, College Park, MD; <sup>2</sup>Johns Hopkins University, School of Medicine, Baltimore, MD; <sup>3</sup>JHU, Bloomberg School of Public Health, Baltimore, MD
- WP 517 A Recovery Strategy of Co-Depleted Proteins in Affinity-Based Separation Workflows for Plasma and serum; Yanbao Yu<sup>1,2</sup>; Harsha P. Gunawardena<sup>1,2</sup>; Xian Chen<sup>1,2</sup>; <sup>1</sup>University of North Carolina, Chapel Hill, NC; <sup>2</sup>UNC-Duke Proteomics Centre, Chapel Hill, NC
- WP 518 Proteomic Analysis of Human Plasma Proteins by IEF-LC-MS/MS Analysis following Depletion of High-Abundance Proteins; Chengjian Tu; Misti Yates; Kristin Cheek; Robbert Slebos; David Tabb; Daniel C.

- Liebler; Department of Biochemistry, Vanderbilt University, Nashville, TN
- WP 519 Enhanced Analytical Resolution Due to Efficient
  Depletion of Albumin and IgG from Human Plasma
  Using New Prepacked Columns; Inger Salomonsson;
  Susanna Lindman; Ulf Hellberg; Staffan Lindqvist;
  Gunnar Glad; Lena Jonsson; Ann Bergh; GE
  Healthcare, Uppsala, Sweden
- WP 520 FT-ICR MS Profiling of Small Molecule Derived from Plasma Obtained from Gaucher Disease Patients; TuKiet T. Lam<sup>1</sup>; Mei Yang<sup>1</sup>; Michael Easterling<sup>2</sup>; Edward Voss<sup>1</sup>; Pramod K. Mistry<sup>1</sup>; Kenneth R. Williams<sup>1</sup>; <sup>1</sup>Yale University, New Haven, CT; <sup>2</sup>Bruker Daltonics, Inc., Billerica, MA
- WP 521 A High Quality Human Plasma Proteome Available in the PeptideAtlas; Terry Farrah<sup>1</sup>; Eric Deutsch<sup>1</sup>; David Shteynberg<sup>1</sup>; David S Campbell<sup>1</sup>; Henry H. Lam<sup>2</sup>; Zhi Sun<sup>1</sup>; Gilbert Omenn<sup>1,3</sup>; Ruedi Aebersold<sup>1,4</sup>; 

  <sup>1</sup>Institute for Systems Biology, Seattle, WA; <sup>2</sup>Hong Kong University of Science and Technology, Clear Water Bay, Hong Kong; <sup>3</sup>University of Michigan, Ann Arbor, MI; <sup>4</sup>Swiss Federal Institute of Technology, Zurich, Switzerland
- WP 522 **Development of Metrics for Assessment of Plasma Quality**; <u>Lisa J Zimmerman</u><sup>1</sup>; Julie A Coleman<sup>1</sup>;

  Douglas P Hardin<sup>1</sup>; Alexander Statnikov<sup>1</sup>; Constantin Aliferis<sup>2</sup>; Daniel C. Liebler<sup>3</sup>; <sup>1</sup>Vanderbilt University, Nashville, TN; <sup>2</sup>New York University, New York, NY; <sup>3</sup>Vanderbilt Univ. School of Medicine, Nashville, TN
- WP 523 **LC-MS/MS Analysis of HDL Complexes Isolated by IgY Immuno-Capture**; <u>Yunan Miao</u><sup>1</sup>; Junji Watanabe<sup>2</sup>;
  George Katselis<sup>1</sup>; Srinivasa T. Reddy<sup>2</sup>; Terry Lee<sup>1</sup>; <sup>1</sup>City of Hope, Duarte, CA; <sup>2</sup>University of California, Los Angeles, Los Angeles, CA
- WP 524 Quantitative Study of Plasma Proteome Dynamics in Genetically Leptin Deficient Patients during Leptin Replacement Treatment; Victor Andreev<sup>2</sup>; Ravi Dwivedi<sup>1</sup>; Gilberto Paz-Filho<sup>2</sup>; Oleg V. Krokhin<sup>1</sup>; Ma-Li Wong<sup>2</sup>; John Wilkins<sup>1</sup>; Julio Licinio<sup>2</sup>; <sup>1</sup>University of Manitoba, Winnipeg, Canada; <sup>2</sup>University of Miami, Miami, FL

# PROTEOMICS: TISSUE, 525 - 560

- WP 525

  iTRAQ Labeling for Tissue Proteomics of Gastric Cancer; Arivusudar Marimuthu<sup>1,2</sup>; Yashwanth Subbannayya<sup>2</sup>; Harsha H.C<sup>1,2</sup>; Santhosh Renuse<sup>2</sup>; Ghantasala S. Sameer Kumar<sup>2</sup>; Manoj K Kashyap<sup>1,2</sup>; Vijayakumar M<sup>3</sup>; Veerendra Kumar K.V.<sup>3</sup>; Vijayalakshmi Deshmane<sup>3</sup>; Girija Ramaswamy<sup>3</sup>; Rekha V Kumar<sup>3</sup>; Raghothama Chaerkady<sup>1,2</sup>; Pradip Kumar Acharya<sup>2</sup>; Akhilesh Pandey<sup>1</sup>; <sup>1</sup>Johns Hopkins University, Baltimore, MD; <sup>2</sup>Institute of Bioinformatics, Bangalore, Karnataka; <sup>3</sup>Kidwai Memorial Institute of Oncology, Bangalore, India
- WP 526 Discovering Novel Components of the Dystrophin-Associated Protein Complex Using Mass Spectrometry-Based Approaches; Aaron Lorsong; Yetrib Hathout; Eric Hoffman; Children's Natl. Medical Center, Washington, DC
- WP 527 Quantitative Proteomics Analysis of Alcohol-Induced Cardiomyopathy Using Label Free LC-MS
  Approache; Elizabeth Yohannes<sup>1</sup>; Helen Anni<sup>2</sup>; Gregory E Gonye<sup>2</sup>; Sergei Ilchenko<sup>1</sup>; Emanuel Rubin<sup>2</sup>; Mark R. Chance<sup>1</sup>; <sup>1</sup>Case Western Reserve University, Cleveland, OH; <sup>2</sup>Thomas Jefferson University, Philadelphia, PA

- WP 528 **2D DIGE Proteomics of Rat Mammary Gland Intact**Proteins to Identify Basis of Anti-Cancer Activity by
  Chemopreventive Polyphenols; Mark B. Cope<sup>1,2</sup>;
  Landon Wilson<sup>1</sup>; Richie Herring<sup>1</sup>; Gloria Robinson<sup>1</sup>;
  Xiangqin Cui<sup>1,2</sup>; Stephen Barnes<sup>1,2</sup>; Helen Kim<sup>1,2</sup>;

  <sup>1</sup>University of Alabama at Birmingham, Birmingham,
  AL; <sup>2</sup>UAB Center for Nutrient-Gene Interaction,
  Birmingham, AL
- WP 529 Uncovering Changes to the Zebrafish Skeletal Muscle Proteome Induced by Hypoxia; Kan Chen; Richard B.

  Cole; Bernard B. Rees; University of New Orleans, New Orleans, LA
- WP 530 Quantitative Analysis of Central Nervous System
  Myelin by NanoUPLC-MSE; Stefan Tenzer<sup>1</sup>; Hauke B
  Werner<sup>2</sup>; Olaf Jahn<sup>2</sup>; Hansjörg Schild<sup>1</sup>; <sup>1</sup>University of
  Mainz, Mainz, Germany; <sup>2</sup>Max Planck Institute of
  Experimental Medicine, Goettingen, Germany
- WP 531 Quantitative Proteomic Profiling Reveals a Role for miR-128 in Prostate Cancer Progression; Arun Sreekumar<sup>1</sup>; Amjad Khan<sup>2</sup>; Laila Poisson<sup>2</sup>; Vadiraja B. Bhat<sup>3</sup>; Rong Zhao<sup>4</sup>; Javed siddiqui<sup>2</sup>; Alexey Nesvizhskii<sup>2</sup>; Gilbert Omenn<sup>2</sup>; Arul Chinnaiyan<sup>4</sup>; 

  <sup>1</sup>Medical College of Georgia, Augusta, GA; <sup>2</sup>University of Michigan, Ann Arbor, Michigan; <sup>3</sup>Agilent Technologies, Wilmington, DE; <sup>4</sup>University of Michigan, Pathology, Ann Arbor, MI
- WP 532 Studying Mammalian Peroxisomes by Quantitative High Resolution Mass Spectrometry; Sebastian Wiese<sup>1</sup>; Thomas Gronemeyer<sup>1</sup>; Rob Ofman<sup>2</sup>; Christian Bunse<sup>1</sup>; Martin Eisenacher<sup>1</sup>; Christian Stephan<sup>1</sup>; Hans R. Waterham<sup>2</sup>; Ronald J.A. Wanders<sup>2</sup>; Helmut E. Meyer<sup>1</sup>; Bettina Warscheid<sup>1</sup>; Ruhr-University Bochum, Bochum, Germany; University of Amsterdam, Amsterdam, The Netherlands
- WP 533 MALDI-MS Analyses of Time-Dependent Changes in Tissue Protein Signals after Ethanol Fixation; Hay-Yan J. Wang; Cheng Bin Liu; Jr Shin Kuo; Hsiao-Han Wang; National Sun Yat-Sen University, Kaohsiung, Taiwan
- WP 534 A Novel Closed ESI Interface Improved LC-MRM Assays for Biomarker Verification on Large-Cell Neuroendocrine Lung Cancer (LCNEC); Toshihide Nishimura<sup>1</sup>; Tetsuya Fukuda<sup>2</sup>; Hiroshi Hike<sup>3</sup>; Kiyonaga Fujii<sup>4</sup>; Hiroko Hamasaki<sup>5</sup>; Masaharu Nomura<sup>1</sup>; Yasuhiko Bando<sup>2</sup>; Norihiko Ikeda<sup>1</sup>; Harubumi Kato<sup>1</sup>; \*\*ITokyo Medical University, Tokyo, Japan; \*\*Pokyo, Japan; \*\*AMR Inc., Tokyo, Japan; \*\*4Hokkaido University, Sapporo, JAPAN; \*\*The University of Tokyo, Tokyo, Japan
- WP 535 Proteomic Profiling of Populus trichocarpa for the Interrogation of Molecular Mechanisms behind Wood Formation; Taufika Islam Williams; Ying-Hsuan Sun; Ting-Feng Yeh; Jason S. Sampson; David C. Muddiman; Vincent Chiang; North Carolina State University, Raleigh, NC
- WP 536 Top-Down High Resolution Electron Capture
  Dissociation Mass spectrometry for Characterization
  of Post-Translational Modifications in Mouse
  Cardiac Troponin; Serife Ayaz Guner<sup>1</sup>; Lin Li<sup>1</sup>; Chris
  Doede<sup>1</sup>; Jeffery W. Walker<sup>1,2</sup>; Ying Ge<sup>1</sup>; <sup>1</sup>University of
  Wisconsin-Madison, Madison, WI; <sup>2</sup>University of
  Arizona, Tucson, AZ
- WP 537 Proteomic Analysis of ADAM17 Metalloproteinase-Cleaved Proteins from PMA-Stimulated Human Platelets; <u>Karen Pei Yi Fong</u><sup>1</sup>; Colin G. Barry<sup>1</sup>; Tilo Grosser<sup>1</sup>; Anh Tran<sup>1</sup>; Hsin-yao Tang<sup>2</sup>; Ian A. Blair<sup>3</sup>;

- David W. Speicher<sup>2</sup>; Lawrence Brass<sup>1</sup>; <sup>1</sup>University of Pennsylvania, Philadelphia, PA; <sup>2</sup>The Wistar Institute, Philadelphia, PA; <sup>3</sup>Univ. of Penn/SOM/Pharmacol, Philadelphia, PA
- WP 538 Quantitative Protein Profiling of Drosophila Parkin Null Mutants Using Stable Isotope Labeling and Label-Free Proteomics; Zhiyin Xun<sup>1</sup>; Thomas C Kaufman<sup>2</sup>; David E. Clemmer<sup>2</sup>; <sup>1</sup>UC-davis, Davis, CA; <sup>2</sup>Indiana University, Bloomington, IN
- WP 539 Proteomic Foray into White Rhinoceros (Ceratotherium simum) Horn Keratin; Stefan Clerens; Santanu Deb-Choudhury; Anita J. Hancock; Charisa D. Cornellison; Jeff E. Plowman; Henning Koehn; Ancy Thomas; Jolon M. Dyer; AgResearch Limited, Christchurch, New Zealand
- WP 540 Identification and Quantification of NMDA Receptor Complex Proteins in Human Postmortem Brain Tissue Samples; Matthew L Macdonald<sup>1</sup>; Eugene F. Ciccimaro<sup>3</sup>; Anamika Banerjee<sup>1</sup>; Chang-gyu Hahn<sup>1</sup>; Ian A. Blair<sup>2</sup>; <sup>1</sup>University of Pennsylvania, Philadelphia, PA; <sup>2</sup>Univ. of Penn/SOM/Pharmacol, Philadelphia, PA; <sup>3</sup>Thermo Fisher Scientific, Somerset, NJ
- WP 541 Quantitative Proteomic Analysis of Diabetic Cardiomyopathy Using Label-free Mass Spectrometry; Chao Yuan<sup>1</sup>; Gregg DiNuoscio<sup>1</sup>; Andrew Keller<sup>2</sup>; Gaurav S.J.B. Rana<sup>1</sup>; Andrea Romani<sup>1</sup>; Mark Chance<sup>1</sup>; <sup>1</sup>Case Western Reserve Univ., Cleveland, OH; <sup>2</sup>Rosetta Biosoftware, Seattle, WA
- WP 542 Identification of Brain Proteins Co-Aggregated with Memapsin 2; Xiaoman Li; Jordan Tang; Univ. of OK Health sci centr, Oklahoma City, OK
- WP 543 GeLC-MS/MS Analysis of Rat Lens Proteins and Associated Effects From Aging/Environment; Kyle A. Floyd; David R. Stella; Landon Wilson; Michael R. Heaven; Stephen Barnes; University of Alabama at Birmingham, Birmingham, AL
- WP 544 **Proteomic Profiling of Rat Heart Aging**; Zongming Fu<sup>1</sup>; Chunling Fan<sup>1</sup>; Lesley Kane<sup>1</sup>; Marjan Gucek<sup>1</sup>; Geoffrey Hesketh<sup>1</sup>; Liqun Jiang<sup>2</sup>; Jing Zhang<sup>2</sup>; Mingyi Wang<sup>2</sup>; Allen Everett<sup>1</sup>; Jennifer Van Eyk<sup>1</sup>; Edward Lakatta<sup>2</sup>; Johns Hopkins School of Medicine, Baltimore, MD; National Institute on Aging, Baltimore, MD
- WP 545 Evaluation of Sample Preparation Methods for Improved Extraction of Membrane Proteins for Effective Proteomic Analysis of Small Number of Cells; Dipak Thakur¹; Tomas Rejtar¹; Buffie Clodfelder-Miller²; Dennis Sgroi³; Barry L. Karger¹; ¹Northeastern University, Boston, MA; ²University of Alabama, Birmingham, AL; ³Massachusetts General Hospital, Charlestown, MA
- WP 546 Quantitative Proteomic Analysis Reveals Redirection of Nuclear-Cytoplasmic Trafficking upon Avian Influenza Infection in Lung Epithelial Cells; Eric Y. Chan; Yu Li; Michael G. Katze; University of Washington, Seattle, WA
- WP 547 Comparison of Human Uridine
  Glucuronosyltransferase Enzyme Expression Levels
  within Human Liver, Intestine and Kidney using
  nanoLC Tandem Mass Spectrometry; David
  Harbourt<sup>1</sup>; John Fallon<sup>1</sup>; Shinya Ito<sup>2</sup>; Takashi Baba<sup>4</sup>;
  Joseph K Ritter<sup>3</sup>; Philip C. Smith<sup>1</sup>; Gary L. Glish<sup>2</sup>; <sup>1</sup>UNC
  Chapel Hill, Chapel Hill, NC; <sup>2</sup>University of North
  Carolina, Chapel Hill, NC; <sup>3</sup>Virginia Commonwealth
  University Medical Center, Richmond, VA; <sup>4</sup>Univ. North
  Carolina, Chapel Hill, NC

- WP 548 Tissue Proteomics: A SILAM-Based Workflow For Targeted Differential Analysis Applied To Sleep Nuclei; Ronald A. Miller<sup>1</sup>; Christopher J. Winrow<sup>1</sup>; Daniel S. Spellman<sup>1</sup>; Rhonda R. Taylor<sup>1</sup>; Duane R. Reiss<sup>1</sup>; James P. Conway<sup>2</sup>; Francisco J. Dieguez-Acuna<sup>1</sup>; John J. Renger<sup>1</sup>; Ronald C. Hendrickson<sup>2</sup>; <sup>1</sup>Merck Research Laboratories, West Point, PA; <sup>2</sup>MRL, Rahway, NJ
- WP 549 Characterization of the Biological Effects of
  Naphthenic Acid Exposure on Zebrafish (Danio
  rerio) Gill Proteome using 2MEGA Stable Isotope
  Labeling; Andrea G. De Souza; Tyson J. MacCormack;
  Andy Lo; Greg G. Goss; Liang Li; University of Alberta,
  Edmonton, Canada
- WP 550 Characterization of Tubulin Isotypes in Human Tumor Tissue; <u>Leah M. Miller</u>; Phyllis M. Novikoff; Susan Band Horwitz; Ruth Hogue Angeletti; *Albert* Einstein College of Med, Bronx, NY
- WP 551 Proteomic Analysis of the Effect of the Gut
  Microbiome on Host Cells; Xinxin Zhang<sup>1</sup>; Nikhil
  Garge<sup>1</sup>; Dallas Donohoe<sup>2</sup>; Sarah Bortvedt<sup>2</sup>; Scott
  Bultman<sup>2</sup>; Maureen K. Bunger<sup>1</sup>; \*\*Research Triangle
  Institute, Research Triangle Park, NC; \*\*University of
  North Carolina-Chapel Hill, Chapel Hill, NC
- WP 552 Large Scale Analysis of Breast Cancer Tissue
  Proteomes Using an Accurate Mass and Time (AMT)
  Tag Approach; V.S. Kumar Kolli¹; Tao Liu²; Brianne
  Petritis²; Luke Weaver¹; Brenda Deyarmin¹; Jennifer
  Kane¹; Richard Katenhusen¹; David Kirchner¹; Karin
  Rodland²; David Camp²; Richard D. Smith²; Craig
  Shriver³; Richard J. Mural¹; ¹Windber Research
  Institute, Windber, PA; ²Pacific Northwest National
  Laboratory, Richland, WA; ³Walter Reed Army Medical
  Center. Washington. DC
- WP 553 **Development of a Reproducible Sample Processing**Method for Quantification of Proteins in Muscle
  Tissue; Ekaterina G. Deyanova<sup>1</sup>; Zhenlian/vivian Ke<sup>2</sup>;
  Kevin Nennig<sup>1</sup>; Yi Du<sup>1</sup>; Kai Zhou<sup>1</sup>; Francisco Dieguez<sup>2</sup>;
  Nathan Yates<sup>1</sup>; Ronald Hendrickson<sup>1</sup>; <sup>1</sup>Merck Research
  Laboratories, Rahway, NJ; <sup>2</sup>Merck, West Point, PA
- WP 554 Cell Type Specific Protein Cataloguing of Barrett's Esophagus: Workflow Design and Evaluation;

  Christoph Stingl<sup>1</sup>; Frederike G.I. van Vilsteren<sup>2</sup>; Coskun Guzel<sup>1</sup>; Theo M. Luider<sup>1</sup>; Jacques J. Bergman<sup>2</sup>;

  Erasmus MC, Rotterdam, The Netherlands; Academic Medical Center, Amsterdam, The Netherlands
- WP 555 Mining the Human Placenta Proteome ≥ 5000
  Proteins Deep Using CID/ETD on a Novel Ion Trap
  Mass Spectrometer; Simone M Lemeer¹; Andrea
  Schneider²; Markus Lubeck³; Bernhard Kuster¹;

  ¹ Technical Universitiy Munich, Freising, Germany;

  ² Bruker Daltonics, Bremen, Germany; ³ Bruker Daltonik
  GmbH, Bremen, Germany
- WP 556 Comparison of First-dimension Separations for "MudPIT" Proteomic Studies on Endometrial Tissue; Steven L. Young<sup>1</sup>; Maria Warren Hines<sup>2</sup>; Nedyalka Dicheva<sup>2</sup>; Mihaela Mocanu<sup>2</sup>; Marc Fritz<sup>1</sup>; Scotchie Jessica<sup>1</sup>; Carol E. Parker<sup>2</sup>; <sup>1</sup>Div. of Reprod. Endocrin. & Infertiility, UNC-CH, Chapel Hill, NC; <sup>2</sup>UNC-Duke Proteomics Center, UNC-CH, Chapel Hill, NC
- WP 557 **MS(E) Differential Proteomic Analysis of Archival**Formalin Fixed, Celloidin Embedded Human Inner
  Ear Tissue; Karin Green<sup>1</sup>; Antti A. Aarnisalo<sup>2</sup>; Jennifer
  O'Malley<sup>2</sup>; Joe Adams<sup>2</sup>; Saumil N. Merchant M.D. <sup>2</sup>;
  James E. Evans<sup>1</sup>; <sup>1</sup>U-MASS Medical School, Worcester,

- MA; <sup>2</sup>Mass. Eye & Ear Infirmary, Harvard Medical School, Boston, MA
- WP 558 Quantitative Proteome Analysis of Slow and Fast
  Skeletal Muscle Tissue Using in vivo SILAC; Marcus
  Krueger¹; Hannes Drexler²; Anne Konzer¹; Aaron
  Ruhs¹; Luca Mendler¹; Thomas Braun¹; <sup>1</sup>MPI for Heart
  and Lung Research, Bad Nauheim, Germany; <sup>2</sup>MPI for
  Molecular Biomedicine, Muenster, Germany
- WP 559 **Tissue-Specific N-Glycopeptide Profiling Maps**; Carey Sheu<sup>1</sup>; Kelly Cooke<sup>1</sup>; David S Campbell<sup>1</sup>; Miyoun Brusniak<sup>1</sup>; Simon Letarte<sup>1</sup>; Julian D Watts<sup>1</sup>; Ruedi Aebersold<sup>1,2</sup>; <sup>1</sup>Institute for Systems Biology, Seattle, WA; <sup>2</sup>ETH Swiss Federal Institute of Technology, Zurich, Switzerland
- WP 560 Quantitative Analysis of Proteomic Changes in Alix Knockout Mice for High-Throughput Profiling of the Regulated Protein Expression by Poorly-Characterized Proteins; Robert Dejournett<sup>1</sup>; Yanbao Yu<sup>1</sup>; Oliver Bogler<sup>2</sup>; Xian Chen<sup>1</sup>; <sup>1</sup>University of North Carolina, Durham, NC; <sup>2</sup>UT M.D. Anderson Cancer Center, Houston, TX

# **METABOLITE PROFILING, 561 - 582**

- WP 561 **Cell Type Classification by Phonotype Specific Markers of Live Single Cells**; <u>Akinori Hosokawa</u>;
  Naohiro Tsuyama; Hajime Mizuno; Takanori Harada;
  Tsutomu Masujima; *Hiroshima Univ. BioMed.*, *Hiroshima, Japan*
- WP 562 What Do We Learn about Hepatotoxicity Using
  Coumarin-Treated Rat Model? Ming-chih D. Ho<sup>1</sup>;
  Bob Xiong<sup>1</sup>; S. Stellar<sup>2</sup>; J. Silva<sup>2</sup>; H. K. Lim<sup>2</sup>; Patrick
  Bennett<sup>1</sup>; Lily Li<sup>1</sup>; J. Proctor<sup>2</sup>; <sup>1</sup>Tandem Labs New
  England, Boxborough, MA; <sup>2</sup>Johnson & Johnson PRD,
  Raritan, NJ
- WP 563 Characterization of Metabolites in Stachybotrys chartarum by LC/TOF-MS; Masahiko Takino<sup>1</sup>; Eri Ochiai<sup>2</sup>; Katsuhiko Kamei<sup>2</sup>; Yoshiko Sugita-Konishi<sup>3</sup>; <sup>1</sup>Agilent Technologies, Hachioji-shi, Japan; <sup>2</sup>Medical mycology reserach Center, Chiba University, Chiba-shi, Japan; <sup>3</sup>National Institute of Health Sciences, Tokyo, Japan
- WP 564 Mass Spectrometric Analysis of Metabolites in Corn (Zea Mays) Root by Mid-Infrared Laser Ablation Electrospray Ionization at Atmospheric Pressure;

  Jennifer A Day; Peter Nemes; Akos Vertes; George Washington University, Washington, DC
- WP 565 Mass Spectrometry Study of Vine Defense Mechanisms Against *Plasmopara viticola*; Gregory Hamm<sup>1</sup>; Benoit Maunit<sup>2</sup>; Anne Poutaraud<sup>3</sup>; Vincent Carré<sup>1</sup>; Didier Merdinoglu<sup>3</sup>; Jean Francois Muller<sup>1</sup>; <sup>1</sup>LSMCL, Metz, France; <sup>2</sup>ICOA, Orléans, France; <sup>3</sup>INRA, Colmar, France
- WP 566 Quantitation of Several HIV Antiretroviral Drugs in Human Plasma by LC Tandem MS; <u>David W. Blank</u>; Brian J. Gilfix; Marcos DiFalco; Line Roy; Bernard F. Gibbs; <u>McGill University</u>, <u>Montreal</u>, <u>Canada</u>
- WP 567 Comprehensive Profiling of Human Plasma
  Phospholipids by Combining Direct Infusion and LC
  FTMS; Rachel Kozlowski; Jun Han; Christoph H.
  Borchers; GBC UVic Proteomics Centre, Victoria,,
  Canada
- WP 568 Identification of Cell Cycle Specific Metabolite
  Profile by Single Cell Mass Spectrometry in NIH3T3
  Cells; Yuka Miho; Naohiro Tsuyama; Hajime Mizuno;
  Takanori Harada; Tsutomu Masujima; Hiroshima Univ.
  BioMed., Hiroshima, Japan

- WP 569 Characterization of Methylated Flavonoid Regioisomers using Tandem Mass Spectrometry;

  Chao Li<sup>1</sup>; Feng Shi<sup>1</sup>; Adam Schmidt<sup>2</sup>; Eran Pichersky<sup>2</sup>;

  A. Daniel Jones<sup>1</sup>; <sup>1</sup>Michigan State University, East Lansing, MI; <sup>2</sup>University of Michigan, Ann Arbor, MI
- WP 570 Spatially Resolved Non-Targeted Metabolic Profiling of Medicago Truncatula and Medicago Sativa Border Cells; Mohamed Bedair<sup>1</sup>; Bonnie S. Watson<sup>1</sup>; Ewa Urbanczyk-Wochniak<sup>2</sup>; David Huhman<sup>3</sup>; Lloyd W. Sumner<sup>4</sup>; Isamuel Roberts Noble Foundation, Ardmore, OK; Monsanto, St. Louis, MO; The Samuel Roberts Noble Foundation, Ardmore, OK; The Noble Foundation, Ardmore, OK
- WP 571 An Unusual Mass Spectrometric Fragmentation
  Pattern of a Group of Sulfonyl Compounds: BetaElimination and Subsequent Retro-Diels-Alder Ring
  Opening; Hlaing (Holly) Maw; Hongbin Yu;
  Boehringer Ingelheim Pharmaceuticals, Inc., Ridgefield,
  CT
- WP 572 Acyl CoA-Profiling in Biological Tissues Using Online SPE-LC-FTMS (Orbitrap); Christoph Magnes<sup>1</sup>; Maria Suppan<sup>1</sup>; Petra Kienesberger<sup>2</sup>; Tarek Moustafa<sup>3</sup>; Thomas Pieber<sup>1,3</sup>; Frank Michael Sinner<sup>1</sup>; I Joanneum Research Forschungsgesellschaft mbH, Graz, Austria; University of Graz, Graz, Austria; Medical Univ. of Graz, Graz, Austria
- WP 573 Lipidomic Profiling of Steroid and Fatty Acid Derivatives Using High-Temperature Gas Chromatography-Mass Spectrometry; Hyun-Jin Jung<sup>1,2</sup>; Won-Yong Lee<sup>2</sup>; Bong Chul Chung<sup>1</sup>; Man-ho Choi<sup>1</sup>; \*Life Sciences Division / KIST, Seoul, South Korea; \*Yonsei University, Seoul, Korea
- WP 574 Quantitative Steroid Signatures by Gas
  Chromatography-Mass Spectrometry for MultipleSubstrate Enzyme Assays; Ju-Yeon Moon<sup>1,2</sup>; Hyun-Jin
  Jung<sup>1,2</sup>; Man-ho Choi<sup>1</sup>; Myeong Hee Moon<sup>2</sup>; Bong Chul
  Chung<sup>1</sup>; \*\*Itife Sciences Division / KIST, Seoul, South
  Korea; \*\*2Yonsei University, Seoul, South Korea
- WP 575 Plant Gibberellins: LC-MS/MS and GC-MS for Profiling, Identification and Quantification; Baichen Zhang<sup>1</sup>; Leslie M. Hicks<sup>2</sup>; <sup>1</sup>Donald Danforth Center, St Louis, MO; <sup>2</sup>Danforth Center, St. Louis, MO
- WP 576 Accelerating Japanese Green Tea Quality Assessment by Ultra Fast LC-IT-TOF MS Based Profiling Studies Using High Mass Accuracy MSn Analysis;

  Tairo Ogura<sup>1</sup>; Takushi Yamamoto<sup>1</sup>; Satoshi Yamaki<sup>1</sup>; Tatsunari Yoshida<sup>1</sup>; Hirohisa Mikami<sup>1</sup>; Rui Kawahara<sup>2</sup>; Takeshi Bamba<sup>2</sup>; Eiichiro Fukusaki<sup>2</sup>; <sup>1</sup>Shimadzu corporation, Kyoto, Japan; <sup>2</sup>Osaka University, Osaka, Japan
- WP 577 Quantitation of Amino Acids in Dried Blood Spots by iTRAQ®Regent Derivatization Reaction and LC/MS/MS Analysis; Songhyun Yang¹; Jungsun Han¹; Chuljin Moon¹; Hansoon Kwon²; Sanghwa Kim²; Jim Krol³; Scott B. Daniels³; Susan Leonard³; ¹Green Cross Reference Laboratory, Yongin, South Korea; ²Applied Biosystems, Seoul, South Korea; ³Applied Biosystems1, Framingham, MA
- WP 578 Embryonic Cell Metabolite Profiling during
  Neuronal Differentiation by Single Cell Mass
  Spectrometry; Naohiro Tsuyama; Hajime Mizuno;
  Takanori Harada; Tsutomu Masujima; Hiroshima Univ.
  BioMed., Hiroshima, Japan
- WP 579 Complementarity of Plasma Proteome and Urinary Metabolome Changes Associated with Extreme Obesity, Metformin Therapy and Bariatric Surgery;

| WP 580   | Stephen B. Harvey; Todd Kellogg; Therese Swan; Gary Nelsestuen; University of Minnesota, Minneapolis, MN Fast HPLC-MS Analysis of Acylcarnitines in Biological Matrices; Paul Minkler; Stephen Ingalls; Charles Hoppel; Case Western Reserve Univ., Cleveland, OH | WP 592  | Chemical Ionization Detection of Haloamines in Real Time Using SIFT-MS; Murray J. Mcewan <sup>1</sup> ; John Gray <sup>2</sup> ; Wan Ping Hu <sup>2</sup> ; Daniel Milligan <sup>2</sup> ; Vaughan Langford <sup>2</sup> ; <sup>1</sup> University of Canterbury, Christchurch, New Zealand; <sup>2</sup> Syft Technologies Ltd, 3 Craft Pl, Christchurch, New Zealand |
|----------|---|---------|--|
| WP 581   | Identification of Cryptorchidism in Horses by Analysing Their Urine Samples with Gas Chromatography Mass Spectrometry; Jenny K.Y. Wong; David K.K. Leung; Francis P.W. Tang; Terence S.M. Wan; The Hong Kong Jockey Club, Hong Kong,                              | WP 593  | GC-Tandem Quadrupole Mass Spectrometry as an Alternative to High-Resolution Mass Spectrometry for the Investigation of Polychlorinated Dioxins and Furans; Anthony Macherone; Agilent Technologies, Elkton, MD   |
| WP 582   | China Measuring the Quantity of Gold Nanoparticles Uptake into Mammalian Cells by Mass  | WP 594  | Comparative Evaluation of Target/Non-Target<br>Screen and Quantitation Techniques of 250 Pesticides<br>in Potable Water; <u>Peter Stone</u> ; Michael Flanagan;  |
|          | Spectrometry; <u>Huan-Chang Lin</u> <sup>1</sup> ; Hsin-Hung Lin <sup>1</sup> ; Cai-Yu Kao <sup>2</sup> ; Alice L. Yu <sup>1</sup> ; Wen-ping Peng <sup>1,2</sup> ; Chung-Hsuan Chen <sup>1</sup> ; <i>Genomics Research Center, Academia Sinica,</i>             | WP 595  | Agilent Technologies, Santa Clara, CA Pharmaceutical Contaminant Screen in Drinking Water and Surface Water by Direct Online Analysis;   |
|          | Taipei, Taiwan; <sup>2</sup> National Dong Hwa University,<br>Shoufeng, Hualien, Taiwan<br>ENVIRONMENTAL, 583 - 609   | WP 596  | Francois A. Espourteille; Catherine Lafontaine; Thermo Fisher Scientific, Franklin, MA Host-Guest Chemistry to Improve LC-MS Detection   |
| WP 583   | Molecular Characterization of Sea-Surface   |         | Limits for Pharmaceuticals Present as Pollutants in Drinking Water; Nirmala Viswanathan; Regina Nardi;   |
|          | Microlayers in the Adriatic Using Fourier Transform<br>Ion Cyclotron Resonance Mass Spectrometry; Boris   |         | Lauren Pettit; David Sierra; <u>Dil Ramanathan;</u> Kean   |
|          | P. Koch <sup>2,3</sup> ; Matthias Witt <sup>1</sup> ; Blazenka Gasparovic <sup>4</sup> ; Sanja  | WD 507  | University, Union, NJ  |
|          | Frka <sup>4</sup> ; Gerhard Kattner <sup>2</sup> ; Christian Albers <sup>1</sup> ; <sup>1</sup> Bruker<br>Daltonik GmbH, Bremen, Germany; <sup>2</sup> Alfred Wegener   | WP 597  | Wastewater Impurity Screening Coming from Large<br>Chemical Plants Using a Combination of Polarity   |
|          | Institute for Polar and Marine Res, Bremerhaven,  |         | Switching ESI & APCI LC-MS/MS Analysis; Markus   |
|          | Germany; <sup>3</sup> University of Applied Sciences,   | WP 598  | Mickel; Applied Biosystems, Darmstadt, Germany LC/TOF-MS for the Analysis of Pharmaceuticals and   |
|          | Bremerhaven, Germany; <sup>4</sup> Ruder Boskovic Institute,<br>Zagreb, Croatia   | W1 370  | their Degradates in Water; Imma Ferrer; Michael  |
| WP 584   | Characterization of Perfluorinated Acids by MALDI-  | WD 500  | Thurman; University of Colorado, Boulder, CO   |
|          | TOF/TOF Mass Spectrometry; Bing Guan <sup>1</sup> ; Joseph B.   | WP 599  | HPLC/MS/MS Characterization of a Putative New Nitrosamine Disinfection By-Product: N-Nitroso-3-  |
|          | Ferrario <sup>2</sup> ; Richard B. Cole <sup>1</sup> ; <sup>1</sup> University of New Orleans, New Orleans, LA; <sup>2</sup> USEPA, Stennis Space Center, MS  |         | Methylindole; Jessica M. Boyd; Feng Qin; Xing-fang   |
| WP 585   | Rapid Analysis of Pharmaceutical Contaminants in  | WD (00  | Li; University of Alberta, Edmonton, Canada  |
|          | Groundwater with Ambient Mass Spectrometry; <u>Ian</u>  | WP 600  | LC-MS/MS Analysis of Selected Perfluorinated Alkyl<br>Acids in Drinking Water, EPA Method 537, a   |
|          | S. Campbell; Alain Ton; Christopher C. Mulligan;<br>Illinois State University, Normal, IL   |         | Validation Study; Jia Wang <sup>1</sup> ; Charles Neslund <sup>1</sup> ;   |
| WP 586   | Fast Screening for Explosives at Ultra-High   |         | Jonathan Beck <sup>2</sup> ; <sup>1</sup> Lancaster Laboratories, Lancaster, PA; <sup>2</sup> Thermo Fisher Scientific, San Jose, CA   |
|          | Resolution: Utilization of Simple Method<br>Development Using a Benchtop Orbitrap Mass  | WP 601  | Low Femtogram Target Screening and Quantitation  |
|          | Spectrometer; <u>Josef Ruzicka</u> ; Kevin J. Mchale; Mark  |         | of Polyfluorinated Compounds (PFCs) in Food  |
| HID 505  | Sanders; Thermo Fisher Scientific, Somerset, NJ   |         | Matrices; Peter Stone <sup>1</sup> ; <u>Linda Cote<sup>2</sup></u> , <sup>1</sup> Agilent Technologies Inc, Santa Clara, CA; <sup>2</sup> Agilent  |
| WP 587   | Dioxin Analysis by Gas Chromatography-Fourier<br>Transform Mass Spectrometry; Vincent Y. Taguchi <sup>1</sup> ;   |         | Technologies, Saint-laurent, QC  |
|          | Ray E. Clement <sup>1</sup> ; Stefan Krolik <sup>3</sup> ; Robert Nieckarz <sup>1,2</sup> ;   | WP 602  | LC-TOF/MS and UPLC-MS/MS Methods for the   |
|          | Robert Williams <sup>4</sup> , <sup>1</sup> Ministry of the Environment,<br>Toronto, ON; <sup>2</sup> University of Waterloo, Waterloo,   |         | Analysis of Perfluorooctanesulfonate (PFOS) and the<br>Reduction of Matrix Interference in Complex   |
|          | Canada; <sup>3</sup> Consultant to Varian Inc, Montreal, Canada;  |         | Biological Matrices; Mark J. Strynar <sup>1</sup> ; Amy D.   |
|          | <sup>4</sup> Varian Inc, Lake Forest, CA  |         | Delinsky <sup>1</sup> ; Andrew B. Lindstrom <sup>1</sup> ; Shoji F. Nakayama <sup>2</sup> ; Jessica L. Reiner <sup>3</sup> ; <sup>1</sup> U.S. EPA NERL, Durham, NC; <sup>2</sup> U.S.   |
| WP 588   | Melamine Screening in Milk Using Low Temperature Plasma Ionization on a Portable Mass Spectrometer;   |         | EPA NRMRL, Cincinnati, OH; <sup>3</sup> NIST Hollings Marine   |
|          | Guangming Huang; Zheng Ouyang; R. Graham Cooks;   |         | Laboratory, Charleston, SC   |
| WD 500   | Purdue University, West Lafayette, IN   | WP 603  | Comparison of Conventional and Low Flow LC-ESI-<br>MS For Analysis of Free and Conjugated Estrogens  |
| WP 589   | Combinatorial Library-Building Based on GC-GC/MS Heartcuts and Spectral Deconvolution to  |         | in Environmental Matrices; Jerry Tso; Diana Aga;   |
|          | Identify Alkylated PAH in Crude Oils; Albert Robbat;  | WD 604  | University at Buffalo, Buffalo, NY   |
| WP 590   | Christian Zeigler; <i>Tufts University, Medford, MA</i> <b>Determination and Reduction of the Effects of</b>  | WP 604  | Dynamic MRM Acquisition Method Optimization for UHPLC-QQQ Multi-Residue Analytical   |
| vv 1 330 | Fragment Ion Interferences in High-Resolution   |         | Applications; Michael Flanagan; Bruce Wang; Harry  |
|          | Environmental Analyses; <u>Jerry Hart</u> ; Carla Lyon; Yves  | WP 605  | Bunting; Agilent Technologies, Santa Clara, CA Multi-Target Screening of up to 500 Pesticides in a   |
| WP 591   | Tondeur; Analytical Perspectives, Wilmington, NC Application of a Novel GC-MS Method for Assessing  | **1 003 | Single LC/MS Run by xact Ion Traces; Petra Decker <sup>1</sup> ;   |
| 271      | <b>Endogenous Metabolites in Exhaled Breath</b>   |         | Marcus Macht <sup>2</sup> ; Arndt Ingendoh <sup>1</sup> ; <u>Laurie Allen<sup>3</sup></u> ;  |
|          | Condensate; Heidi F Hubbard; Joachim D Pleil; Jon R   |         | <sup>1</sup> Bruker Daltonik GmbH, Bremen, Germany; <sup>2</sup> Bruker  |
|          | Sobus; Michael C Madden; US EPA, Rtp, NC  |         |  |

- Daltonics GmbH, Bremen, Germany; <sup>3</sup>Bruker Canada Inc., East Milton, Canada
- WP 606 Single Step LC-MS Method for the Simultaneous
  Determination of Organochlorine and Phenoxy Acid
  Pesticides; Giorgio Famiglini; Pierangela Palma;
  Elisabetta Pierini; Veronica Termopoli; Helga Trufelli;
  Achille Cappiello; Università di Urbino, Urbino, Italy
- WP 607 The Use of MRM and MRM3 Mode for Rapid
  Analysis of Iodinated X-Ray Contrast Media; Jan
  Lembcke<sup>1</sup>; Birgit von Oepen<sup>2</sup>; <sup>1</sup>Applied Biosystems,
  Darmstadt, Germany; <sup>2</sup>Hamburgwasser, Hamburg,
  Germany
- WP 608 Using Bonded Silica Solid Phase Microextraction Fibers as a Screening Tool for Pharmaceuticals and Personal Care Products in Drinking Water; Carmen T. Santasania; Katherine Stenerson; Robert Shirey; An Trinh; Craig Aurand; Supelco/Sigma-Aldrich, Bellefonte, PA
- WP 609 **Hyphenated Techniques as Modern Detection**Systems in Ion Chromatography; Jörg Kleimann;
  Stefanie Czyborra; Andrea Wille; Metrohm AG,
  Herisau, Switzerland

# **POLYMERS, 610 - 630**

- WP 610 Qualitative and Quantitative Determination of Cellulose Polymer Derivatives Using Size-Exclusion Chromatography and ELSD-MS Detection; Louisphilippe Labranche<sup>1</sup>; Audrey Tousignant<sup>3</sup>; Yves G. Leblanc<sup>2</sup>; Alain Carrier<sup>2</sup>; Sandoz, Boucherville, Canada; Sandoz Canada, Boucherville, QC; Sandoz Canada Inc., Boucherville, QC
- WP 611 On-Line Coupling of Liquid Chromatography at Critical Conditions with Electrospray Tandem Mass Spectrometry for the Structural Characterization of Block Copolymers; Marion Girod; Trang N.T. Phan; Laurence Charles; University Aix-Marseille I & III, Marseille Cedex 20, France
- WP 612 LC-MS of EO-PO Block Copolymers Using
  Ultrasonic Degradations and the Mechanism of
  Degradation; Ryuichi Arakawa<sup>1</sup>; Masanori
  Okabayashi<sup>1</sup>; Takehiro Watanabe<sup>1</sup>; Yukari Nishimoto<sup>2</sup>;
  Tomoyuki Ozawa<sup>3</sup>; Hideya Kawasaki<sup>1</sup>; <sup>1</sup>Kansai
  University, Osaka, Japan; <sup>2</sup>Nippon Synthetic Chemical
  Industry, Osaka, Japan; <sup>3</sup>Nissan Chemical Industries,
  Chiba, Japan
- WP 613 Characterization of the Physical and Chemical Networks in Filled Rubber Compounds by Pyrolysis GC/MS; Alesia Salberg<sup>1</sup>; Abdulkareem Melaiye<sup>2</sup>; Ed Johnson<sup>2</sup>; Chrys Wesdemiotis<sup>1</sup>; \*\*Ithe University of Akron, Akron, OH; \*\*The Goodyear Tire & Rubber Company, Akron, OH
- WP 614 Comprehensive Two Dimensional Liquid
  Chromatography/Mass Spectrometric (LCxLC/MS)
  Analyses for Characterization of Solid Epoxy Resins;
  Samir Julka; Hernan Cortes; Bob Harfmann; Bruce Bell;
  Andreas Schweizer-Theobaldt; Matthias Pursch; David
  West; Shawn Maynard; Dow Chemical Company,
  Mildland, MI
- WP 615 Characterization of Povidones in Ophthalmic
  Solution by GPC-ELSD / LC-MS Analysis; Audrey
  Tousignant<sup>1</sup>; Louis-philippe Labranche<sup>3</sup>; Yves G.
  Leblanc<sup>1</sup>; Alain Carrier<sup>2</sup>; \*Isandoz Canada Inc.,
  Boucherville, Canada; \*Isandoz Canada, Boucherville,
  OC; \*Isandoz, Boucherville, OC
- WP 616 Collision Induced Dissociation Processes in Azofunctional Oligoesters; Cristian Peptu<sup>1</sup>; Valeria Harabagiu<sup>2</sup>; Bogdan C. Simionescu<sup>2</sup>; Marek

- Kowalczuk<sup>1</sup>; <sup>1</sup>Jan Dlugosz University, Czestochowa, Poland; <sup>2</sup> "Petru Poni" Institute, Iasi, Romania
- WP 617 Solvent Effect on the DESI Mass Spectra of Industrial Polymers and Additives; Matthieu Loriau<sup>1</sup>; Sandra Alves<sup>1</sup>; Florence Churlaud<sup>2</sup>; Jean-Claude Tabet<sup>1</sup>; Iniversity Paris VI (UPMC), Paris Cedex O5, France; Arkema CERDATO, Serquigny, France
- WP 618 MALDI Characterization of Polymers Using
  Accurate Mass Measured Data for Accelerated
  Material Understanding; Sean Bennett<sup>1</sup>; Sucharita
  Dutta<sup>1</sup>; William Nichols<sup>2</sup>; Andrew J. Hoteling<sup>2</sup>; <sup>1</sup>Thermo
  Fisher Scientific, San Jose, CA; <sup>2</sup>Eastman Kodak
  Company, Newark, NY
- WP 619 Characterization of Poly(organophosphazene)s by Mass Spectrometry Techniques; Vincenzo Scionti; Claire Tessier; Wiley Youngs; Chrys Wesdemiotis; The University of Akron, Akron, OH
- WP 620 Derivatization Strategies for Improved MALDI Mass Spectrometry of MAA-MMA Copolymers; Rémi Giordanengo<sup>1</sup>; Stéphane Viel<sup>1</sup>; André Thévand<sup>1</sup>; Laurence Charles<sup>1</sup>; Béatrice Allard-Breton<sup>2</sup>; IUniversity Aix-Marseille I & III, Marseille Cedex 20, France; <sup>2</sup>ARKEMA, Pierre-Bénite, France
- WP 621 Overcoming the Limitations of MALDI-TOF-MS
  Analysis of Polymers Using GPC-MALDI and a
  Hybrid Ion Trap Time of Flight MALDI MS; Brian
  Feild<sup>1</sup>; Fan Xiang<sup>2</sup>; Martin Resch<sup>3</sup>; Chrys Wesdemiotis<sup>4</sup>;

  Shimadzu, Columbia, MD; Shimadzu Biotech,
  Pleasanton, CA; Shimadzu Europe, Duisburg,
  GERMANY; The University of Akron, Akron, OH
- WP 622 Comparative Study of Fatty Alcohol Alkoxylate
  Copolymers Fragmentation Patterns by MALDIMS/MS Using Low Energy and High Energy CID;
  Volker Wulf¹; Martin Resch²; Oliver J. Schmitz¹; HansWilli Kling³; Siegmar Gaeb¹; Michaela Wirtz³;

  ¹University of Wuppertal, Wuppertal, Germany;
  ²Shimadzu Europe, Duisburg, Germany; ³Cognis GmbH,
  Duesseldorf, Germany
- WP 623 End-Group Determination in Minor Components of Polyalkylene Glycoles by MALDI-ToF Mass Spectrometry Following Preliminary Derivatization; Roman Borisov; Nikolai Yu. Polovkov; Vladimir Zaikin; Topchiev Institute of Petrochemical synthesis, Moscow, Russian Federation
- WP 624 Identification of Functional Additives in
  Polybutadiene by Tandem Mass Spectrometry; David
  E. Dabney; Jon Janoski; Roderic P. Quirk; Chrys
  Wesdemiotis; The University of Akron, Akron, OH
- WP 625 Quantitation of PEG Contaminants in Ethoxylated Surfactant Samples by MALDI TOFMS Using Standard Additions and Internal Standards Methods; Scott D. Hanton<sup>2</sup>; Diane M. Henning<sup>3</sup>; Kevin G. Owens<sup>1</sup>; Renata Szyszka<sup>1</sup>; <sup>1</sup>Drexel University, Philadelphia, PA; <sup>2</sup>Air Products & Chemicals, Inc., Allentown, PA; <sup>3</sup>Air Products and Chemicals, Inc., Milton. WI
- WP 626 **Positive and Negative Mode Mass Spectrometry of Poly(electrolytes)**; Bethany Subel<sup>1</sup>; Chrys
  Wesdemiotis<sup>2</sup>; <sup>1</sup>University of Akron, Akron, OH; <sup>2</sup>The
  University of Akron, Akron, OH
- WP 627 Mass Spectrometry of Polyethylene Glycols:

  Evidence of Structural And Energetic

  Interdependence; Antony Memboeuf<sup>1</sup>; Ron M.A.

  Heeren<sup>2</sup>; Andreas Nasioudis<sup>3</sup>; Oscar F. Van Den Brink<sup>4</sup>;

  Karoly Vekey<sup>5</sup>; Laszlo Drahos<sup>1</sup>; hungarian Academy Of Sciences, Budapest, Hungary; <sup>2</sup>FOM Inst.

- Atomic/Molecular Phy, Amsterdam, Netherlands; <sup>3</sup>AkzoNobel, Arnhem, Netherlands; <sup>4</sup>Akzo Nobel, Utrecht, Netherlands; <sup>5</sup>Hungarian Academy of Science, Budapest, Hungary
- WP 628 Development of a Novel Analytical Technique for the Identification of Organic Contamination on Spaceflight-Related Substrates Utilizing a DART-TOF; Kathleen Brooks Loftin<sup>1</sup>; Timothy P. Griffin<sup>2</sup>; Christian A. Clausen III<sup>3</sup>; <sup>1</sup>NASA- Kennedy Space Center, Kennedy Space Center, FL; <sup>2</sup>NASA, Kennedy Space Center, FL; <sup>3</sup>University of Central Florida, Orlando, FL
- WP 629 Characteristic Fragmentation of Polysiloxanes in Monolayer by Monoatomic and Polyatomic Ions Bombardment in ToF-SIMS; Hye Kyoung Moon; David D. Wells; Joseph A. Gardella; SUNY Buffalo, Buffalo, NY
- WP 630 Surface Analysis of Polyacetylene Thin Films by UV-LDI-FTMS; Sasa Miladinovic<sup>1</sup>; Valérie De Vriendt<sup>2</sup>; Scott A. Robotham<sup>3</sup>; Stéphane Lucas<sup>2</sup>; Charles L. Wilkins<sup>1</sup>; <sup>1</sup>University of Arkansas, Fayetteville, AR; <sup>2</sup>University of Namur-PMR, Namur, Belgium; <sup>3</sup>Nebraska Wesleyan University, Lincoln, NB

# **HYDROCARBON AND PETROCHEMICAL, 631 - 659**

- WP 631 Matrix Optimization for the MALDI-TOF-MS
  Analysis of Biodiesel Components; Casey R.

  Mcalpin<sup>1,2</sup>; Kent J. Voorhees<sup>1</sup>; Robert L. McCormick<sup>2</sup>;
  Teresa L. Alleman<sup>2</sup>; <sup>1</sup>Colorado School of Mines, Golden,
  CO; <sup>2</sup>National Renewable Energy Laboratory, Golden,
- WP 632 Working Toward a Petroleomic Analysis of Bio-oils; Erica Smith<sup>1,2</sup>; David Perdian<sup>1,2</sup>; Young Jin Lee<sup>1,2</sup>; \*\*Department of Chemistry, Iowa State University, Ames, IA; \*\*2Ames Laboratory- U.S. DOE, Ames, IA
- WP 633 Characterization of Sterol Glucosides Found in B100 Biodiesels by Gas and Liquid Chromatography/Mass Spectrometry; Ryan Shea; Rick Pauls; BP Chemicals, Naperville, IL
- WP 634 MALDI-TOF MS Screening of Aged Biofuels; <u>Julie Herniman</u><sup>1</sup>; G. John Langley<sup>1</sup>; Tom Lynch<sup>2</sup>; <sup>1</sup>University of Southampton, Southampton, UK; <sup>2</sup>BP Castrol Global Lubricants Technology, Pangbourne, UK
- WP 635 Biodiesel Identification: Distinguishing individual Fatty Acid Methyl Esters and Identifying Oxidation Products Using MS Coupled to Chromatographic Techniques; Christianne Wicking<sup>1</sup>; G. John Langley<sup>1</sup>; Tom Lynch<sup>2</sup>; <sup>1</sup>University of Southampton, Southampton, UK; <sup>2</sup>BP Castrol Global Lubricants Technology, Pangbourne, UK
- WP 636 Identification of Oxidation Products of Biodiesel under Accelerated Oxidation Condition; Jungju Seo<sup>1</sup>; Myung Hee Nam<sup>1</sup>; Manhoi Hur<sup>3</sup>; Jae-Kon Kim<sup>2</sup>; Mi-Jin Lee<sup>1</sup>; <sup>7</sup>Korea Basic Science Institute, Seoul, South Korea; <sup>2</sup>Korea Institute of Petroleum Quality, Ochangeup, Korea; <sup>3</sup>BNF Technology Inc, Daejeon, Korea
- WP 637 Analysis of Carbohydrates and Lipids in Microalgal Biomass Samples with HPAEC-MS and LC/MS;

  Linda Lopez<sup>1</sup>; Ting Zheng<sup>1</sup>; Rodney Corpuz<sup>2</sup>; Rosanne Slingsby<sup>1</sup>; Srinivasa Rao<sup>1</sup>; \*Dionex Corporation, Sunnyvale, CA; \*General Atomics, San Diego, CA
- WP 638 Ionization Techniques and Reagents for Improved Heteroatom Speciation in Crude Oils by Ultrahigh Resolution FT-ICR MS; Privanka Juyal<sup>1,2</sup>; Amy Mckenna<sup>4</sup>; Ryan P. Rodgers<sup>3</sup>; Alan G. Marshall<sup>5</sup>; <sup>1</sup>Nalco Company, Sugar Land, TX; <sup>2</sup>Nat'l High Magnetic Field Laboratory, Tallahassee, FL; <sup>3</sup>Nat'l High Magnetic

- Field Lab, Tallahassee, FL; <sup>4</sup>Natl High Magnetic Field Laboratory, Tallahassee, FL; <sup>5</sup>Ion Cyclotron Resonance Prog, Tallahassee, FL
- WP 639 Identification, Characterization and Quantitation of Vanadyl Porphyrins in Heavy Crude Oil by FT-ICR Mass Spectrometry; Ryan P. Rodgers<sup>1</sup>; Jeremiah M. Purcell<sup>2</sup>; Amy Mckenna<sup>1</sup>; Alan G. Marshall<sup>1</sup>; <sup>1</sup>Nat'l High Magnetic Field Laboratory, Tallahassee, FL; <sup>2</sup>Shell Global Solutions, Houston, TX
- WP 640 Exploring Solvent and Concentration Effects on Average Molecular Weight (MW) Data for Petroleum Samples using Electrospray Ionization Mass Spectrometry (ESI-MS); Melisa Clements; Thomas Oldenburg; Steve Larter; PRG, University of Calgary, Calgary, Canada
- WP 641 Identification of Chemical Components in Shale Oils by ESI and APPI Fourier Transform Ion Cyclotron Resonance Mass Spectrometry; Eun Suk Park<sup>1</sup>; Jeol Geol Na<sup>2</sup>; Soo Hyun Chung<sup>2</sup>; Manhoi Hur<sup>4</sup>; Hojoon Seo<sup>4</sup>; Sunghwan Kim<sup>3</sup>; Young Hwan Kim<sup>1</sup>; Jong Shin Yoo<sup>1</sup>; <sup>1</sup>Korea Basic Science Institute, Chungwon-kun, Chungbuk-do, South Korea; <sup>2</sup>Korean Institute of Energy Research, Daejeon, South Korea; <sup>3</sup>Korean Basic Science Institute, Ochang-myun, SOUTH KOREA; <sup>4</sup>BNF Technology Inc., Daejeon, South Korea
- WP 642 Isolation and Characterization of Naphthenic Acids in Crude Oils by Electrospray Ionization FT-ICR Mass Spectrometry; Mmilili Myles Mapolelo<sup>1</sup>; Ryan P. Rodgers<sup>2</sup>; Alan G. Marshall<sup>3</sup>; \*Iforida State Univ, Dept of Chemistry, Tallahassee, FL; \*Nat'l High Magnetic Field Lab, Tallahassee, FL; \*Ion Cyclotron Resonance Prog. Tallahassee, FL
- WP 643 Analysis of Fresh and Used Lubricating Oils Using
  ASAP in Conjunction with Ion Mobility Mass
  Spectrometry; Hilary J. Major<sup>1</sup>; Martin Selby<sup>2</sup>; Martin
  Green<sup>1</sup>; Alistair Wallace<sup>1</sup>; Waters Corporation,
  Manchester, UK; Shell Global Solutions (UK), Chester,
  UK
- WP 644 Identification of Low Abundant Impurities in Gas Oil by Fourier Transform Ion Cyclotron Resonance Mass Spectrometry; Matthias Witt; Jochen Friedrich; Bruker Daltonik GmbH, Bremen, Germany
- WP 645 The Effect of Operating Conditions on Petroleum
  Analysis by Fourier Transform Ion Cyclotron
  Resonance Mass Spectrometry; Haiyan Wang; Gil
  Jones; Matthew Unterfenger; Victor Kovar; Howard
  Greenberg; Hung Pham; Stella Cabanban; Paul Adams;
  Andrzej Ringwelski; UOP LLC, A Honeywell Company,
  Des Plaines, IL
- WP 646 Geochemical Applications of Electron Ionization GC-MS with Supersonic Molecular Beams; David A.

  Zinniker¹; Pierre Metzger²; J. Michael Moldowan¹;
  Alexander B. Fialkov³; Aviv Amirav⁴; ¹Stanford
  University, Stanford, CA; ²Ecole Nationale Supérieure
  de Chimie de Paris, Paris, France; ³Tel Aviv University,
  Tel Aviv, ISRAEL; ⁴Tel-Aviv University, Tel-aviv,
  ISRAFI
- WP 647 Element Speciation in Petroleum and Petroleum Products by HPLC-ICP MS; Guilhem Caumette<sup>1,2</sup>; Charles-Philippe Lienemann<sup>1</sup>; Isabelle Merdrignac<sup>1</sup>; Brice Bouyssiere<sup>2</sup>; Ryszard Lobinski<sup>2</sup>; <sup>1</sup>IFP Lyon, Vernaison, France; <sup>2</sup>LCABIE CNRS UMR 5254, Pau, France
- WP 648 Development of an Analytical Protocol to Investigate Solid Well Bore Deposits: Determination of Heterocyclic Compounds by FT-ICR MS; <u>Saroj</u>

- Panda<sup>1</sup>; Jan T. Andersson<sup>2</sup>; Wim Genuit<sup>3</sup>; Mark Grutters<sup>3</sup>; Andrew G. Shepherd<sup>3</sup>; Wolfgang Schrader<sup>1</sup>; 

  <sup>1</sup>Max-Planck Inst Coal Res., Mülheim / Ruhr, Germany; 

  <sup>2</sup>Inst. Inorg. and Analytical Chem, Univ. Muenster, 
  Muenster, Germany; <sup>3</sup>Shell Global Solutions, 
  Amsterdam, Netherlands
- WP 649 Investigations into Asphaltene Molecular-Mass
  Distribution and Plasma-Phase Aggregation Using
  Two-Step Laser Mass Spectrometry and LDI-MS;
  Amy L. Morrow<sup>1</sup>; Andrew E. Pomerantz<sup>2</sup>; Matthew R.
  Hammond<sup>1</sup>; Oliver C. Mullins<sup>2</sup>; Richard N. Zare<sup>1</sup>;

  \*\*Istanford University, Stanford, CA; \*\*Schlumberger-Doll Research, Cambridge, MA\*\*
- WP 650 GCxGC TOF MS and Electrospray FT-ICR-MS
  Identification of Asphaltene Precipitate
  Componments Understanding Water-In-Oil
  Emulsion Stability; Brendan F Graham<sup>2</sup>; Eric F. May<sup>2</sup>;
  Robert Trengove<sup>1</sup>; Murdoch University, Murdoch,
  Australia; University of Western Australia, Crawley,
  Australia
- WP 651 Evidence of Paraffin Traping by Asphaltenes
  Detected by LDI TOF MS; Brice Bouyssiere<sup>3</sup>; Socrates
  Acevedo<sup>1</sup>; Ryszard Lobinski<sup>3</sup>; Josmelith M. Cordero T.

  <sup>1</sup>; Hervé Carrier<sup>2</sup>; <sup>1</sup>Universidad Central de Venezuela,
  Caracas 1053, Venezuela; <sup>2</sup>Laboratoire des Fluide
  Complexe, Univeristé de Pau, Pau, France; <sup>3</sup>LCABIE CNRS/UPPA UMR 5254, Pau, France
- WP 652 **Observation of Fullerenes from PAH's in MALDI TOF**; Robert E. Haufler<sup>2</sup>; Alexandre Loboda<sup>2</sup>; L. P.
  Felipe Chibanta<sup>1</sup>; Brad McCann<sup>1</sup>; <sup>1</sup>University of New
  Brunswick, Fredericton, Canada; <sup>2</sup>MDS Analytical
  Technologies, Concord, Canada
- WP 653 **REMPI Measurements of Aromatics in Hydrocarbon Model Flames**; <u>Tina Kasper</u>; Nils Hansen; *Sandia Nat. Labs.*, *CRF*, *Livermore*, *CA*
- WP 654 Compositional Analysis of Petroleum Distillation Residue by APCI FT-ICR Mass Spectrometer;

  Eunkyoung Kim<sup>1,1</sup>; Myoung-han No<sup>1,2</sup>; Jaesuk Koh<sup>1,2</sup>; Sunghwan Kim<sup>1,3</sup>; Manhoi Hur<sup>1,4</sup>; <sup>1</sup>, Daejeon, South Korea; <sup>2</sup>SK energy Institute of Tech., Daejeon, South Korea; <sup>3</sup>Korean Basic Science Institute, Ochang-myun, South Korea; <sup>4</sup>BNF Technology, 556, Youngsan-dong, Yuseong-gu, Daejeon, South Korea
- WP 655 Molecular Analysis of a Coal Liquefaction Product by FT-ICR/MS – Comparison of ASAP, ESI, APCI and APPI Ionization Techniques; Jeremie Ponthus; Lyes Assam; Institut Français du Petrole, Solaize, France
- WP 656 What Color Is Your Fuel Spill? Solvent Dyes in Fuels and Fuel Spill Samples by Electrospray Ionization Mass Spectrometry; Colleen Rostad; USGS, WRD, NRP, Lakewood, CO
- WP 657 The Petroleome: A Mass Spectral Database of Petroleum Composition; Jade Velasquez<sup>1,3</sup>; Amy Mckenna<sup>1,2</sup>; Ryan P. Rodgers<sup>1,2</sup>; Alan G. Marshall<sup>1,2</sup>; 

  <sup>1</sup>Natl High Magnetic Field Laboratory, Tallahassee, FL; 
  <sup>2</sup>Department of Chemistry and Biochemistry, FSU, Tallahassee, FL; 
  <sup>3</sup>Florida State University, Tallahassee, Florida
- WP 658 Statistical Interpretation of Crude Oil High Resolution Spectra Obtained by ESI and APPI FT-ICR Mass Spectrometry Using Principal Components Analysis; Manhoi Hur¹; Somi Shin¹; Hojoon Seo¹; InJoon Yeo²; Eun Suk Park²; Eunkyoung Kim³; Myoung-han No³; Young Hwan Kim²; Sunghwan Kim²; 

  \*\*BNF Technology Inc., Daejeon, South Korea; \*\*ZKorea\*\*

- Basic Science Institute, Chungwon-kun, Chungbuk-do, South Korea; <sup>3</sup>SK energy Institute of Tech., Daejeon, South Korea
- WP 659 The Analysis of Mass Spectra in Petroleomics A
  Novel Application for Machine Learning; Jennifer
  Hauschild; Hugh Cartwright; University of Oxford,
  Oxford, UK

# ION STRUCTURES / ENERGETICS, 660 - 677

- WP 660 Structural Characterization of Gas-phase Uranyl Trihalide Anions Using IRMPD Spectroscopy; Gary Groenewold<sup>2</sup>; Michael Kullman<sup>1</sup>; Ryan Dain<sup>1</sup>; Jos Oomens<sup>3</sup>; Jeffrey Steill<sup>3</sup>; Michael J. Van Stipdonk<sup>1</sup>; 

  <sup>1</sup>Wichita State University, Wichita, KS; <sup>2</sup>Idaho National Laboratory, Idaho Falls, ID; <sup>3</sup>FOM Rijnhuizen, Nieuwegein, Netherlands
- WP 661 Measuring Infrared "Fingerprint" Spectra of Gas-Phase Zwitterions Using a Continuous Wave OPO Laser; Warren K Mino Jr; Jan Szczapanski; David H. Powell; John R. Eyler; Nicolas Polfer; University of Florida, Gainesville, FL
- WP 662 IRMPD Spectroscopy Investigation of Gas-Phase Sodium and Potassium Chlorate Anions; Ryan P.

  Dain¹; Christopher M. Leavitt¹; Jos Oomens²; Jeffrey Steill²; Gary Groenewold³; Michael J. Van Stipdonk¹;

  Wichita State University, Wichita, KS; ²FOM
  Rijnhuizen, Nieuwegein, Netherlands; ³Idaho National Laboratory, Idaho Falls, ID
- WP 663 **Photoelectron Spectroscopy of Substituted Phenylnitrenes**; Neloni Wijeratne; Paul G. Wenthold;
  Purdue University, West Lafayette, IN
- WP 664 Potassium Affinity of Gas-Phase Amino Acids
  Determined by IRMPD (CO<sub>2</sub>- and Free Electron
  Laser) and Molecular Modeling; Miriam Drayss<sup>1</sup>;
  Frank Dreiocker<sup>1</sup>; Dirk Blunk<sup>1</sup>; Jeremiah M. Purcell<sup>3</sup>;
  Chris Hendrickson<sup>2,6</sup>; Alan G. Marshall<sup>2,6</sup>; Jos Oomens<sup>4</sup>;
  Abhingya Mookherjee<sup>5</sup>; Peter B. Armentrout<sup>5</sup>; Mathias
  Schaefer<sup>1</sup>; Inst. Organic Chemistry University of
  Cologne, Koeln, Germany; Ion Cyclotron Resonance
  Prog, Tallahassee, FL; Shell Global Solutions,
  Houston, TX; FOM Rijnhuizen, Nieuwegein,
  Netherlands; University of Utah, Salt Lake City, UT;
  National High Magnetic Field Laboratory, Tallahassee,
  FI
- WP 665 Chain Length and Sequence Effects on Metal-Ion Peptide Binding Conformations. IRMPD Spectroscopic Exploration; Robert C. Dunbar<sup>1</sup>; Jeffrey Steill<sup>2</sup>; Nicolas Polfer<sup>3</sup>; Jos Oomens<sup>2</sup>; <sup>1</sup>Case Western Reserve Univ, Cleveland, OH; <sup>2</sup>FOM Rijnhuizen, Nieuwegein, Netherlands; <sup>3</sup>University of Florida, Gainesville, FL
- WP 666 The Structure of (M+H-H2O)+ Generated from Protonated Tetraglycine Revealed by Tandem MS and IRMPD Spectroscopy; Michael J. Van Stipdonk<sup>1</sup>; Benjamin Bythell<sup>2</sup>; Ryan Dain<sup>1</sup>; Jos Oomens<sup>3</sup>; Jeffrey Steill<sup>3</sup>; Gary Groenewold<sup>4</sup>; Bela Paizs<sup>5</sup>; <sup>1</sup>Wichita State University, Wichita, KS; <sup>2</sup>GermanCancer Research Center, Heidelberg, Germany; <sup>3</sup>FOM Rijnhuizen, Nieuwegein, Netherlands; <sup>4</sup>Idaho National Laboratory, Idaho Falls, ID; <sup>5</sup>DKFZ, Heidelberg, Heidelberg, Germany
- WP 667 **Structure and Fragmentation Behavior of Metal- Cationized Phosphopeptides**; Sarah M. Young<sup>1</sup>; Sam Molesworth<sup>1</sup>; Jeffrey Steill<sup>2</sup>; Ryan Dain<sup>1</sup>; Jos Oomens<sup>2</sup>; Gary Groenewold<sup>3</sup>; Michael J. Van Stipdonk<sup>1</sup>; <sup>1</sup>Wichita State University, Wichita, KS; <sup>2</sup>FOM Rijnhuizen,

- Nieuwegein, Netherlands; <sup>3</sup>Idaho National Laboratory, Idaho Falls, ID
- WP 668 An IRMPD Study of Radical Cations of Aromatic Amino Acids and their Precursors; Chi-kit Siu¹; Udo Verkerk¹; Junfang Zhao¹; Yuzhu Guo¹; Yuyong Ke¹; Jeffrey Steill²; Jos Oomens²; Robert C. Dunbar³; Alan C. Hopkinson¹; K W Michael Siu¹; ¹CRMS, York University, Toronto, ON; ²FOM Rijnhuizen, Nieuwegein, Netherlands; ³Case Western Reserve Univ, Cleveland, OH
- WP 669 Characterization of the Conformations of Gas-Phase Peptide Ions via Acid-Base Measurements: A Study of Ion Internal Solvation; Jianhua Ren; Kiran Kumar Morishetti; Robert Harper; John Tan; Betty Huang; University of the Pacific, Stockton, CA
- WP 670 Structure and Behavior of Mixed Serine Clusters:
  Molecular Dynamics, Post-Hartree Fock and Density
  Functional Theory Studies; Anthony Costa; R. Graham
  Cooks; Purdue University, West Lafayette, IN
- WP 671 Conformational and Thermochemical Properties of Deprotonated Amino Acid Clusters from High Pressure Mass Spectrometry; Robert J. Nieckarz<sup>1</sup>; Chad G. Atkins<sup>2</sup>; Opal Courtney<sup>1</sup>; Terry Mcmahon<sup>1</sup>; 

  <sup>1</sup>University of Waterloo, Waterloo, Canada; <sup>2</sup>Memorial University, St Johns, Canada
- WP 672 Mechanisms of Characteristic Phospholipid Anion Fragmentations: Theoretical Study II; <u>Daryl Giblin</u>; Fong-Fu Hsu; John Turk; Michael L. Gross; <u>Washington</u> University, St Louis, MO
- WP 673 Mobile Protons and Mobile Radicals: Insights from Time- and Collision Energy-Resolved Surface-Induced Dissociation Studies; Julia Laskin<sup>1</sup>; Zhibo Yang<sup>2</sup>; Ngor Wai Lam<sup>3</sup>; Ivan K. Chu<sup>4</sup>; <sup>1</sup>Pacific NW National Laboratory, Richland, WA; <sup>2</sup>University of Colorado at Bo, Boulder, CO; <sup>3</sup>HKU, Hong Kong, Hong Kong; <sup>4</sup>University of Hong Kong, Hong Kong
- WP 674 **Determination of the Binding Energy of Benzene- Water Cluster**; <u>Laura Haupert</u>; Paul G. Wenthold;

  Purdue University, West Lafayette, IN
- WP 675 Double Hydrogen Transfer on Unimolecular Dissociation for N-(2-Indancarbonyl)-1-azacycloalkan(e)-2-(thi)one Derivatives Including Deuterium Labeled Ones Using a Four Sector Tandem Mass Spectrometer; Hiroshi Yamaoka¹; Kazuo Fujii¹; Rie Uemura¹; Kimio Isa²; Ryuji Nakata²; Tetsuya Maekawa²; Nico M.M. Nibbering³; ¹Osaka Prefecture University, Sakai, Osaka, Japan; ²University of Fukui, Fukui, Japan; ³Vrije Universiteit, Amsterdam, The Netherlands
- WP 676 Selective Bond Breaking in Prompt and Metastable Decay of Deprotonated Monosaccharides the Role of Intramolecular Vibrational Redistribution; Oddur Ingolfsson; Ilko Bald; University of Iceland, Reykjavik, Iceland
- WP 677 Unusual Rearrangements and Fragmentations of different Steroid Ethers upon Electrospray and Electron Ionization; Jurgen Grotemeyer; Christorph Freudenhammer; Christian-Albrechts-Univ, Kiel, Germany

# **COMPUTER APPLICATIONS, 678 - 697**

WP 678

Sub-Part-Per-Million Mass Accuracy Using a Single
Internal Calibrant on an Orbitrap Mass
Spectrometer for Large-Scale Protein Analysis; Craig
D. Wenger; Graeme C. McAlister; Qiangwei Xia; Joshua
J. Coon; University of Wisconsin, Madison, WI

- WP 679 Efficient Validation and Qualification of Mass Spectrometry Systems in a GLP- and GMP-Regulated Environment; Cynthia A. Palmer<sup>1</sup>; Douglas James<sup>2</sup>; Mario Rocci<sup>2</sup>; <sup>1</sup>FDA, Philadelphia, PA; <sup>2</sup>Prevalere Life Sciences, Inc., Whitesboro, NY
- WP 680 **Making a Spectrum Viewer with Microsoft's Windows Presentation Foundation;** Tom Patterson;
  nScan, Medford, MA
- WP 681 Bayesian Tools for Mapping Accurate Mass
  Measurements to Elemental Formulae; Philip C.
  Price<sup>1</sup>; Megan E. Price<sup>3</sup>; Daniel O. Price<sup>2</sup>; The Dow
  Chemical Company, South Charleston, WV; Fellow,
  American Statistical Assoc., Jacksonville, FL; The
  Benetech Initiative, Palo Alto, CA
- WP 682 **Is Wikipedia the Public Face of Mass Spectrometry?**<u>Thabiso Musapelo;</u> Kermit K. Murray; *Louisiana State Univ., Baton Rouge, LA*
- WP 683 An Improved Calibration Method for the MALDI-FTICR Analysis of <sup>15</sup>N-Metabolically Labeled Proteome Digests Using a Mass Difference Approach; LiJing; Jon Amster; University of Georgia, Athens, GA
- WP 684 Image Enhancement with Constraints in the Input Space for ToF/DL Imaging Mass Spectrometry; Andriy Kharchenko; Leendert Klerk; Ron Heeren; FOM Institute for Atomic and Molecular Physics, Amsterdam, Netherlands
- WP 685 Open Access Tables of Accurate Precursor Ion Mass Values for Mass-Based Classification (MBC) of Chemical Compounds; Bernhard Spengler; Alfons Hester; University of Giessen, Giessen, Germany
- WP 686 The IUPAC International Chemical Identifier and Mass Spectrometry; Peter J. Linstrom<sup>1</sup>; Steve R. Heller<sup>1</sup>; Alan D. McNaught<sup>2</sup>; Yuri A. Mirokhin<sup>3</sup>; Stephen E. Stein<sup>1</sup>; Dmitrii V. Tchekhovskoi<sup>1</sup>; <sup>1</sup>NIST, Gaithersburg, MD; <sup>2</sup>IUPAC, Research Triangle Park, NC; <sup>3</sup>KT Consulting, Antioch, CA
- WP 687 Scalable Data Management on a High Throughput MALDI TOF Mass Spectrometer; George Mills; Matthew Gabeler-lee; Virgin Instruments Corporation, Sudbury, MA
- WP 688 Simulation of Ion Transport from Atmospheric Pressure through Intermediate Pressure to Vacuum; Peter Williams; Agilent Laboratories, Santa Clara, CA
- WP 689 Mass++ is a Plug-In Type Universal Freeware for Viewing and Manipulating Large Scale LC/MS Data;

  Satoshi Tanaka<sup>1</sup>; Ken Aoshima<sup>1,2</sup>; Yuji Miura<sup>1,2</sup>;

  Yoshiya Oda<sup>1,2</sup>; <sup>1</sup>CREST, Saitama, Japan; <sup>2</sup>Eisai Co.,

  Ltd, Tsukuba, Japan
- WP 690 Automated Classification of Unknown Biocompounds Using Tandem MS; Sebastian Böcker; Thomas Zichner; Florian Rasche; Friedrich-Schiller-University Jena, Jena, Germany
- WP 691 Optimized Data Compression Strategy for Efficient Storage and Analysis for High Throughput Multidimensional Separations and Mass Spectrometry; Nathaniel Beagley; Chad Scherrer; Yan Shi; Brian H. Clowers; William F. Danielson; Anuj Shah; Anoop M. Mayampurath; Gordon Anderson; Richard D. Smith; Pacific Northwest National Laboratory, Richland, WA
- WP 692 A Peptide Mass Fingerprinting Approach to Enhance Protein Sequence Coverage Using High Mass Accuracy MS1 Spectra; Yunhu Wan; Stefani Thomas; Zhongping Liao; Sarah Rnyarzewski; Nandakumar Madayiputhiya; Noble Nemieboka; Austin Yang; University of Maryland, Baltimore, MD

- WP 693 Developing Application Software Using Applied Biosystem Mass Spectrometer and Shimadzu HPLC to Achieve Multiplexing and Direct Instrument Control in Bioanalysis; Leimin Fan<sup>1</sup>; Richard Koeritz<sup>3</sup>; Tawakol El-Shourbagy<sup>2</sup>; Huaiqin Wu<sup>2</sup>; <sup>1</sup>Abbott Labs, Abbott Park, IL; <sup>2</sup>Abbott Laboratories, Abbott Park, IL; <sup>3</sup>Shimadzu Scientific Instruments Inc., Columbia, MD
- WP 694 Automated Identification of Fragments via Rigorous Statistical Modelling of LC-MS Metabolomic Data;

  Andreas Ipsen; Elizabeth J Want; Timothy M Ebbels;

  Imperial College London, London, UK
- WP 695 Directed Sample Interrogation Utilizing an Accurate Mass Exclusion-Based Data-Dependent Acquisition Strategy (AMEx); Emily Rudomin<sup>2</sup>; Steven A. Carr<sup>2</sup>; Jacob D. Jaffe<sup>1</sup>; <sup>1</sup>The Broad Institute of Ha, Cambridge, MA; <sup>2</sup>Broad Institute, Cambridge, MA
- WP 696 A High Throughput LC/MS/MS Data Analysis
  Approach for Discovery PK and in-vitro BioAnalysis; Mei Foong Hwang; Monica Wu; Mark Gao;
  Quincey Wu; XenoPort, Inc., Santa Clara, CA
- WP 697 The Protein Information and Property Explorer: a Rich-Client Web Application for the Management and Functional Exploration of Proteomic Data;

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